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Demonstrating the Feasibility of Using the 1996 MVP Tracer Study for Transport and Diffusion Model Validation

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Abstract

The 1996 USAF Model Validation Study (MVP) provides an extensive atmospheric tracer database containing over two hundred gaseous tracer releases covering three seasons for the Cape Canaveral Air Force Station (CCAFS). Tracer experiments included both ground-level as well as elevated releases of SF_6. Both puff and continuous releases were conducted.

This report describes a demonstration of the feasibility of using the 1996 MVP study to develop a model simulation database to support the evaluation of the performance of (1) numerical weather prediction models as well as (2) transport and diffusion models, both used to assess potential accident scenarios which might pose a threat from an atmospheric release of hazardous materials near the CCAFS. For this demonstration, the community state-of-the-science Weather Research Forecast (WRF) numerical model was used to develop the meteorological fields used to drive NOAA/ARL's Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) transport and diffusion model.

For this demonstration, Trials 308 and 309, conducted May 1, 1996, from Session Three of the MVP were evaluated.

The demonstration focused on implementation of the WRF model, version 3.8.1, to generate meteorological data to drive HYSPLIT simulations of two MVP tracer releases. Three nested domains were configured in horizontal grid spacing of 27 km, 9 km, and 3 km. In order to increase the influence of sounding observations collected at Cape Canaveral during the tracer experiment on the WRF modeling, sensitivity tests were conducted by (1) conducting the WRF simulation using a default nudging coefficient (labeled “run1”). (2) increasing the nudging coefficient for the wind speed to 8.0e-4 (labeled as “run2”), (3) using 1.2e-3 nudging coefficient for the wind (labeled as “run3”), (4) decreasing the vertical weighting of surface data (labeled as “run4”, and (5) using the Shin-Hong PBL scheme (labeled as “run5”). It was determined that using a larger nudging coefficient for the wind reduced the wind bias. By decreasing the vertical weighting of surface data (run4), the wind speed prediction was nudged closer to the sounding data than the “run2” and “run3” cases. The HYSPLIT results using the “run4” nudging configuration and the “run5” Shin-Hong PBL scheme produced the smallest wind speed bias among the four sensitivity tests.

The NOAA/ARL HYSPLIT model was exercised for both MVP Trials 308 and 309 using the above suite of WRF outputs. Transport and diffusion model predictions were compared to Trial 308 observed tracer measurements between 18.75 and 19.25 km downwind of the elevated release point. Differences between predicted and observed concentrations were found to decrease from roughly a factor of ten underprediction to roughly a factor of three underprediction with the adjustment of WRF from no observational nudging to nudging with both surface and upper air measurements. While Trial 309 reported no measurable ground-level concentrations, aircraft sampling of elevated plumes provided an opportunity to evaluate predicted and measured plume trajectories.

While only a small set of MVP tracer releases were reviewed, it was concluded that given appropriate numerical weather simulation, the 1996 MVP Study could provide a rich database for evaluation, verification, and validation of numerical modeling of the potential release of airborne materials within the CCAFS environment. The MVP study also provides additional opportunities to enhance current scientific understanding of the PBL and convection formulations underpinning current atmospheric transport and dispersion tools addressing the special circumstances of elevated releases.

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1.0 Introduction

The 1995-1997 Model Validation Program (MVP) (Lundblad, 1998; Abernathy, 1999; Kamada, 1997) was initiated by the United States Air Force (USAF) Titan space program over concerns with safety and launch constraints developed from plume predictions associated with rocket launches from the Cape Canaveral Air Force Station (CCAFS) and Vandenberg Air Force Base (VAFB). The MVP goal was to create a large database of plume sampling of tracer gas and supporting meteorological data that can be used to verify and validate plume predictions from diffusion models used at both launch sites. In particular, the SF_6 atmospheric-tracer program focused on plume rise and ground-level concentration predictions of the Rocket Exhaust Environmental Diffusion Model (REEDM), an Eulerian Gaussian plume model, which, at the time, was the basic diffusion predictive model at CCAFS for estimating population exposure to releases of hazardous materials.

During the MVP (Depiction 1) gaseous atmospheric tracer (SF_6) was released into the seasonally prevailing wind conditions which varied from calm to almost 13 m/s and nearly all wind directions. Tracer was released from a free-flying piloted powered blimp typically stationed over CCAFS Tower 110 which is located between Launch Complex 40 (LC-40) and Launch Complex 41 (LC-41). Typical release rates varied from 15-20 kg/hour. Release trials were performed between 5 am and midnight local daylight savings time (GMT-4). While the primary release location was located over CCAFS Tower 110, the release site was sometimes varied to account for shifting synoptic wind conditions such as off-shore flows.

SF_6 was sampled in real time using Scientech TGA-4000 electron capture fast gas analyzers mounted in six vans and two aircraft. Coupled with direct SF_6 gas sampling, plume and puffs were also remotely tracked and imaged with multiple ground-based real-time visible/infrared (IR) cameras using narrow band filters intended to maximize the SF_6 return emission signal.

Meteorological support for MVP included the extensive Cape Canaveral real-time Weather Interactive Network Display (WIND) tower network consisting of 46 instrumented towers. Additional meteorological monitoring was available through a 50 MHz Tropospheric Doppler Radar Wind Profiler (TDRWP) reporting the vertical wind structure between 2000 meters and 18000 meters AGL. A series of RASS-equipped 915 MHz doppler wind profilers provided Planetary Boundary-Layer (PBL) winds and temperature.

Trials 308 and 309 from Session Three on May 1, 1996 were selected for an initial demonstration of the potential for current meteorological and diffusion simulation capabilities to model the Cape Canaveral meteorological conditions for the 1995-1997 tracer release time period, as well as the transport and diffusion of released material. For the demonstration, regional meteorological conditions were simulated with the Weather Research Forecast (WRF, Powers et al. 2017) model initialized with the North American Regional Reanalysis (NARR) and the regional meteorological information provided by the extensive CCAFS monitoring previously described. The three-dimensional mass consistent National Oceanic and Atmospheric Administration Air Resources Laboratory (NOAA/ARL) Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) transport and diffusion model was used to simulate the spread of tracers and subsequent downwind concentrations.

Section 2 of this report outlines the simulation background of the May 1, 1996 MVP tracer trials 308 and 309. Section 3 provides a description of the HYSPLIT model, the WRF model output provided to HYSPLIT to drive the simulated transport and diffusion processes, and the mobile SF6 tracer measurements, while Section 4 presents the HYSPLIT simulations for both tracer trials and is an initial exploration of the skill score associated with HYSPLIT simulations for Trials 308 and 309. A summary of the initial testing and evaluation process is given in Section 5.

2.0 Simulation Background

There are three components for this scoping study exploring the use of the MVP data for model verification and validation. In this case, verification is defined to included testing and evaluation of both the numerical weather prediction model as well as the transport and diffusion model. Validation is defined as the basic ability, through a skill score, of simulations of the meteorological conditions driving the diffusion simulation as well as the basic ability of the diffusion model to predict ground-level concentrations. The three components are the WRF numerical weather prediction model, the HYSPLIT transport and diffusion model, and the MVP tracer experiments which included both tracer release and tracer sampling. These three components are briefly discussed in the following subsections.

2.1 WRF Numerical Weather Prediction Methodology

The WRF model was used to generate meteorological data to drive HYSPLIT for the tracer simulation. Three nested domains were configured with horizontal grid spacing of 27 km, 9 km, and 3 km. The domains have 20 vertical layers within the PBL with the first mid-layer height of the model at approximately 8 m. The initial conditions (IC) and lateral boundary conditions (LBC) for the WRF simulation originated from the North American Regional Reanalysis (NARR). The WRF model was initialized every day at 1800 UTC, and the first 6 hours of spin up time in the 30-h simulation were discarded. The physics options used in the WRF runs included the single-moment 3-class scheme for microphysics, the Rapid Radiative Transfer Model for longwave radiation, the Dudhia scheme for shortwave radiation, the Grell–Freitas ensemble for the subgrid cloud scheme, and the unified Noah land surface model. For the PBL parameterization, WRF simulations used the Mellor-Yamada-Nakanishi-Niino (MYNN) 2.5 level scheme or the Shin-Hong PBL scheme. The lower boundary forcing for vertical transport was from the MYNN surface layer scheme or the Fifth Generation Penn State/NCAR Mesoscale Model (MM5) Monin-Obukhov surface scheme, respectively.

For reducing model bias during the simulation, four-dimensional data assimilation (FDDA), or nudging, is a well-known and efficient method available in the WRF model. Surface and sounding observations were used for improving the reanalysis data for IC/LBC through the objective analysis package available in the WRF model system (Deng et al. 2009). The nudged configuration ingested the improved IC/LBC files and ran with surface and observational nudging in addition to the grid nudging. The variables for nudging are temperature, wind speed, and wind direction. The source of surface and sounding data is the National Center for Atmospheric Research (NCAR) Computational and Information Systems Laboratory Research Data Archive (https://rda.ucar.edu/). An additional source of data is available from the MVP tracer study at CCAFS, which provided spatially and temporally varying dense surface and sounding data during the study period. The use of wind and temperature observations reduces the growth of model errors through observational nudging, which further has a positive impact on the tracer diffusion simulation (Hegarty et al 2013; Ngan and Stein, 2017). Sensitivity tests on the observational nudging parameters were conducted in this study to tailor the nudging configuration for maximizing the influence of sounding data on the model wind field.

2.2 HYSPLIT Transport and Diffusion Modeling

Simulation of the transport and diffusion of the MVP SF_6 tracer release was accomplished with the NOAA/ARL HYSPLIT model (Stein, 2015). HYSPLIT is a complete system for computing air parcel trajectories as well as complex transport, diffusion, chemical transformation, and deposition simulations. Model calculations are based on a hybrid approach between using a Lagrangian frame of reference for the advection and diffusion calculation and Eulerian frame of reference methodology, which uses a fixed frame of reference to compute air concentrations over a fixed three-dimensional computational grid. The HYSPLIT system has continuously improved over the past 30 years from estimating simplified single particle trajectories based on atmospheric radiosonde soundings to a system accounting for multiple interacting pollutants which are transported, dispersed, and deposited over scales ranging from local to global. With respect to the Cape Canaveral environment, HYSPLIT was the model chosen to develop the Environmental Impact Statement (EIS) (FEIS, 2014) and mission risk analysis (SAR/SER) for NASA's Mars 2020 Mission (INSRP, 2019a).

2.3 MVP SF_6 Tracer Measurements and Analysis

For this initial assessment, two tracer trials were selected from the MVP data base. Table 1 provides a summary of the trials which includes tracer release time, location, and height, as well as wind speed and wind direction occurring during the trials. Trials 308 and 309 are from MVP Session Three, conducted on Julian Day 122, May 1, 1996. Both trials represent elevated releases with mean heights of 305m and 610m, respectively. The goal for Trial 308 was to acquire data during an early morning (6:00 am EDT) release in the upper portion of the surface boundary layer to observe the onset and development of inversion breakup fumigation through the morning in response to surface heating. The goal of Trial 309 was to acquire data from a late-morning through early afternoon release in the upper boundary layer to examine mixing to the ground with transport over land, but parallel to the Banana River lagoon shoreline.

2.3.1 Blimp Tracer Releases and Flight Path

Figure 1 plots SF_6 release rates for the Trial 308 and Trial 309 tracer releases from the blimp platform. For both tracer releases, the release rate was set at 18 kg/hour and monitored continuously by a mission scientist on board the blimp. The excursion in the release rate at release startup and end are inconsequential. Figure 2 plots the blimp platform release altitude for each trial with time. As shown in Figure 2, the release height varied by as much as +/- 100m throughout each of the trials. The excursions in the release altitude at release startup and end are also inconsequential. For both Trial 308 and Trial 309, release heights were intended to be located near the top of the developing PBL; the proximity of the release platform to the top of the developing PBL generated significant turbulence for the blimp platform. In order to maintain a reasonable release location, the blimp was forced to fly figure eight flight patterns. Figure 3 presents a map of the flight path for each of the two trials illustrating that the blimp was able to reasonably maintain its latitude/longitude position over the designated release point. Positioning deviations were minimal and should not meaningfully contribute to measured fluctuations in ground-level or airborne measured concentrations. Flight paths are presented on this scale in Figure 3 to illustrate the relative minor deviations of tens of meters in flight trajectories compared to the tens of kilometers scale associated with tracer sampling as illustrated in Figure 4.

2.3.2 SF_6 Samplers and Aircraft and Van Sampling Tracks

Ground-level concentrations for each tracer trial were measured with sampling platforms on vans and aircraft equipped with near real-time (i.e., 1 Hz) SF_6 samplers, as shown in Table 2. Both platforms deployed Scientech TGA-4000 electron capture SF_6 samplers (https://www.arl.noaa.gov/wp_arl/wp-content/uploads/documents/Summaries/Dispersion_Tracer.pdf).

Of the available six instrumented sampling vans, at least five of the vans were deployed during each tracer release. Based on the weather forecast ahead of each tracer release and the predicted plume paths, each of these vans were assigned specific strategic sampling routes on local and regional highways. Vans and aircraft sampled SF_6 along each designated circuit over the entire tracer period.

Aircraft sampling was conducted with Piper Seminole and Navajo Chieftain instrumented aircraft operated by the Florida Institute of Technology. Sampling goals for the aircraft, after plume detection, was to conduct multiple cross-section traverses to define the vertical extent of the released tracer.

Figures 4 and 5 show the sampling paths for both vans and aircraft for tracer trials 308 and 309, respectively. As shown, the sampling vans followed the regional highways with predefined sampling tracks based on projected plume trajectories ahead of the tracer release. Sampling tracks were based on analyses of the current meteorological conditions from the extensive CCAFS and MVP arrays of surface and upper air atmospheric measurements and weather monitoring. Each figure is annotated with the mean wind speed and wind direction assigned to each trial.

2.3.3 Tracer Measurements from Van Sampling

Each van completed multiple traverses along its designated sampling route throughout the 2-hour tracer release period. Sampling routes ranged from 3km - 40 km downwind of the release point. Vans followed available roads crisscrossing the anticipated plume trajectory at 3-4 downwind ranges as illustrated in Figure 4 for Trial 308 and Figure 5 for Trial 309. For both trials, Van 2 was not operational and only one aircraft was available.

It should be noted that moving sampling platforms presents challenges for the analysis of acquired concentration measurements. As shown in Figure 6, during Trial 308 the sampling route of Van 1 and Van 4 followed the Indian River Lagoon Scenic Highway (Route A1A – 528) from the intersection of North Cocoa Beach Blvd to Jetty Park. Figure 7 plots the downwind distance from the tracer release for Van 1 through the Trial 308 sampling period. Van 1 conducted 14 passes through the ground-level tracer concentration field over the roughly 2-hour period during which SF_6 was released from the blimp platform. Figure 8 plots Trial 308 measured $\log_{10}$ concentration in g/m^3 by Van 1 throughout the approximate 2-hour sampling period. As shown in Figure 1, Trial 308 had a constant release rate of 18.0 kilograms per hour through the release period. Given the near-neutral atmospheric conditions for Trial 308 (i.e., moderate to strong winds), the centerline concentration should be expected to be near constant at near-field distances for the core period of the release.

2.3.4 Tracer Measurements from Aircraft Sampling

Aircraft 1 flew multiple paths to detect the released plume as shown in Figure 4. Following plume detection, the aircraft flew sampling trajectories at multiple heights to estimate the vertical depth of the tracer release. This vertical sampling was accomplished for at least three downwind distances.

Analyses of MVP aircraft SF_6 measurements are particularly challenging due to constant location changes of the measuring platforms. As shown in Figure 9, for Trial 308 aircraft sampling plume transects were designed to first locate the released plume and then attempt to define the depth of the dispersing cloud. Short sampling transects were conducted at multiple heights to locate a possible plume centerline and then potentially define a mean SF_6 concentration as a function of height. As indicated in Figure 4, fight paths coincided with mobile ground-level sampling efforts.

Figure 10 plots measured SF_6 concentrations during Trial 308 by the Aircraft 1 sampling transects. Aircraft measurements should, at a minimum, be considered instantaneous observations. Beyond defining plume boundaries, significant analysis is needed to extract verification and validation concentrations for transport and diffusion model comparison. For this assessment, Trial 308 and Trial 309 aircraft measurements are used to qualitatively access the released tracer plume.

3.0 WRF and HYSPLIT Simulations

To explore the feasibility of using the 1996 MVP tracer releases for transport and diffusion model evaluation and validation, two components need to be tested. The first component is the model used to simulate the complex regional and local meteorology fields, and the second component is the transport and diffusion model. Construction of the meteorological database used to drive the transport and diffusion simulations was accomplished using the community state-of-the-science numerical weather prediction model weather research model, WRF. The WRF model local and regional predictions were evaluated against observed meteorological fields using various combinations of data assimilation and numerical PBL schemes as described in Section 2.1. The second component, the transport and diffusion model, was addressed with the state-of-the-science transport and diffusion model HYSPLIT, as described in Section 2.2. HYSPLIT was evaluated for its ability to assimilate WRF simulations and predict the downwind transport and diffusion of MVP tracer releases.

3.1 WRF simulations

The local and regional meteorological conditions supporting analysis of tracer simulations were developed using the advanced research dynamic core of the WRF model. WRF, version 3.8.1, was configured for three nested domains with horizontal grid spacing of 27 km, 9 km, and 3 km. A total of 33 vertical layers were defined with a higher resolution near the surface, and 100 hPa for model top. There were 20 layers below 850 hPa (~1.5 km) with the first mid-layer height of the model at around 8 m. ICs and LBCs for the WRF simulation originated from the NARR (Mesinger et al. 2006). The model was initialized every day at 1800 UTC, and the first six hours of spin-up time in the 30-hour simulation were discarded. The physics options used in the WRF runs included the single-moment 3-class scheme for microphysics, the Rapid Radiative Transfer Model (RRTM) for longwave radiation, the Dudhia scheme for shortwave radiation, the Grell–Freitas ensemble for the subgrid cloud scheme, and the unified Noah land surface model. Two PBL schemes and their corresponding surface schemes were used: (1) the MYNN 2.5 level PBL scheme with the MYNN surface layer scheme; and, (2) the Shin-Hong PBL scheme with the MM5 Monin-Obukhov surface scheme. The former is based on the Total Kinetic Energy (TKE) prediction approach and the other on the first-order diagnostic K-profile parameterization.

Grid and observational nudging were applied to the WRF simulation. The nudging adjusts model values toward observations (i.e., observational nudging) or toward analysis fields (i.e., grid or analysis nudging) at each integration time step. In this study, the nudging was applied to temperature and wind during the simulation to minimize the error growth of these variables. Table 3 shows WRF runs conducted for this study. Each numerical simulation represents an increased complexity in both the level of assimilated meteorological observations as well and the complexity of the WRF simulation. This scheme was designed to test whether WRF could produce the level of meteorological data required to drive HYSPLIT transport and diffusion calculations to model the 1996 MVP tracer releases. The WRF simulation (labeled as “run1”) used the surface and sounding data from the NCAR Computational and Information Systems Laboratory Research Data Archive (https://rda.ucar.edu/)and an additional dataset available from the MVP tracer experiment at Cape Canaveral, which provided a dense surface and sounding data spatially and temporally during the study period. Sensitivity tests were conducted: increasing nudging coefficient for the wind to 8.0e-4 (labeled as “run2”); using 1.2e-3 nudging coefficient for the wind (labeled as “run3”); decreasing the vertical weighting of surface data (labeled as “run4”); and using the Shin-Hong PBL scheme (labeled as “run5”) instead of the MYNN 2.5-level PBL scheme as employed in “run4” and all other simulations.

The best description of the level of agreement between WRF numerical simulation and observations is provided in Figure 11. This plot compares predicted wind speed and wind direction for 11Z and 14Z, 05/01/1996 with Cape Canaveral radiosonde soundings conducted in support of the two May 1, 1996 tracer releases.

In the subsequent discussion of HYSPLIT simulations, the designated WRF (“run5”) numerical simulation was used to drive the HYSPLIT’s transport and diffusion predictions.

3.2 HYSPLIT simulations

MVP Trials 308 and 309 tracer releases were simulated with the NOAA/ARL HYSPLIT transport and diffusion model. For both events, HYSPLIT was configured with SF_6 release rates set at 18 kg/hour for an approximate 120-minute release. For Trials 308 and 309, release heights were set to the nominal latitude and longitude coordinates as well as elevation reported for SF_6 tracer released from the free-flying piloted powered blimp stationed at nominal heights of 305 meters, and 610 meters, respectively.

For each simulation, a total of 250,000 computational particles were used to simulate the released tracer. The sampling grid spacing was set at 0.0005 degrees with a total of 10 degrees set for both latitude and longitude domains. Following the HYSPLIT parameterization scheme developed for the Mars 2020 launch accident risk assessment, the TKE turbulence scheme was selected, with the probabilistic deposition option. Simulation duration was set at 120 minutes with tracer sampling beginning at the initial release time and ending at the termination of the tracer release. HYSPLIT was set to output average concentration fields at the end of the two-hour tracer release period.

While additional model simulations were conducted with varying sampling periods and alternative turbulence and deposition routines, significant variations in predicted concentrations were only attributable to variations in the meteorological database used to drive HYSPLIT's transport and diffusion processes. The set of nine HYSPLIT simulations for Trials 308 and 309 are listed in Table 4.

The initial series of HYSPLIT simulations (i.e., tests 1-3) using the version of HYSPLIT (i.e., Subversion [SVN] 951) employed for the Mars 2020 launch accident risk assessment were conducted to explore differences in transport and diffusion model predictions based solely on the complexity of the numerical weather prediction simulations used to generate the meteorological fields. Additional HYSPLIT simulations (i.e., tests 4-9) using Version 5 of HYSPLIT were intended to resolve differences associated with the version of nudging and the PBL parameterization used to drive the HYSPLIT simulations.

After testing both the older (SVN 951) and newer versions (Version 5 dated 4/1/2020) of HYSPLIT, is was determined to use the newer version. Therefore, unless indicated otherwise, HYSPLIT Version 5 was used for the assessment documented in this report. After additional review, the HYSPLIT option VINIT, which assigns atmospheric turbulence to the initial release was set to zero because allowing VINIT to operate produced an unrealistic expansion of the predicted HYSPLIT ground-level concentration fields.

Figures 12 and 13 present maps of the HYSPLIT predicted 6-hour average ground-level concentrations for Trial 308 and Trial 309, respectively. Figures 14 and 15 plot the predicted 6-hour average concentration at release height for Trial 308 and 309, respectively. In each of these plots, for simplicity in the Geographical Information System (GIS) analysis and clarity of presentation, the $\log_{10}$ of calculated concentrations in g/m^3 is shown.

4.0 Discussion

The following discussion will primarily focus on Trial 308 which has both measurable ground-level and elevated airborne concentrations for comparison with HYSPLIT simulations. While Trial 309 will be briefly introduced, there were no measurable ground-level concentrations observed by the sampling vans. As mapped in Figure 5, for Trial 309, sampling vans and aircraft were staged to observe a forecasted tracer plume with a predicted significant westerly component. In addition, it appears that van sampling was initiated before the tracer would reach measurable ground-level concentration levels as sampling vans simply followed predicted sampling circuits that did not intersect the released plume. Also, while the sampling aircraft was able to locate the released plume, concentrations were near detection limits. Notwithstanding, the Trial 309 aircraft measurements do provide for a limited verification of HYSPLIT's predicted plume trajectory.

4.1 Trial 308

As described in Table 1, Trial 308 was a SF_6 tracer release from a free-flying piloted powered blimp platform flying at 305m AGL located over CCAFS Tower 110. The release rate was 18 kg/hour for approximately 120 minutes. Ground level concentrations were measured by five sampling vans traveling two distinct anticipated plume transects following Route A1A and the Banana River Causeway (as shown in Figure 4).

4.1.1 Trial 308 Ground-level concentration evaluation

Figures 16 shows the ground-level predicted coupled with measured ground-level airborne concentrations for Trial 308. The measurement tracks are highlighted. However, given the relative agreement between modeled and observed concentrations, the color designations for the measurements tend to blend in with the background predictions. Estimates of predicted and measured plume centerlines based on visual interpretation of Figure 16 would suggest a rough 10 to 15 degrees azimuth separation between the two trajectories.

Figures 17 and 18 plot Trial 308 measured as well as simulated ground-level airborne concentrations for two quite different turbulence parameterization techniques. Predicted concentrations in Figure 17 correspond to HYSPLIT predictions compared to Van 1 measured concentrations based on a basic WRF prediction without significant nudging applied based on local and regional weather observations. Predicted concentrations displayed in Figure 18 were developed using the run5 WRF model output to drive HYSPLIT. Those predicted and measured concentrations falling within a 0.5 km band between 18.75 and 19.25 km downwind are plotted. This corresponds to the predicted and observed data point along Route A1A the sampling path performed by Vans 1 and 4.

As noted above, the HYSPLIT predicted plume varies from the observed track by roughly 10 to 15 degrees azimuth. The difference between predicted and measured plume paths is quite typical (Hanna, 1988). As opposed to a potentially misleading direct comparison between offset predicted versus measured concentrations, it is useful to compare predicted and measured concentration levels at generalized downwind travel distances. As indicated above, centerline directional differences do not allow for a robust direct comparison between paired predicted and observed concentration levels. In this evaluation, plotted measured and predicted concentrations were measured (blue) or predicted (red) between 18.75 km and 19.25 km downwind of the release point. The range corresponds to the sampling transect for vans 1 and 4 described in Figure 6. As shown in Figure 17, peak ground-level concentrations predicted by HYSPLIT differ from observed values by roughly an order-of-magnitude for this case. In both cases, HYSPLIT underpredicts.

As discussed in Section 3.1, nine combinations of the WRF numerical weather prediction model and HYSPLIT were generated using increasingly complex PBL parameterizations and degrees of numerical nudging. One numerical modeling advantage offered with the MVP program was access to the extensive atmospheric monitoring program maintained by the US Air Force 45th Weather Squadron (now Space Force) during the period of the MVP Program. For Trial 308, observations from 41 surface monitoring stations, four radar wind/temperature boundary-layer sounders, and two upper-air radiosonde sounding stations were included in the MVP archives.

The wind speed was underpredicted in comparison to sounding data even though all available observations were nudged for the entire simulation as shown by the grey line in Figure 11, labeled as "run1". In order to increase the influence of sounding data collected at Cape Canaveral during this tracer experiment, additional WRF sensitivity tests were conducted as follows:

- "run2" - increasing nudging coefficient for the wind to 8.0e*-4.
- "run3" - using 1.2e*-3 nudging coefficient for the wind.
- "run4" - decreasing the vertical weighting of surface.
- "run5" - using Shin-Hong PBL scheme.

As shown in Figure 18, using a larger nudging coefficient for the wind reduced the wind bias. By decreasing the vertical weighting of surface data ("run4"), the wind speed prediction was nudged closer to the sounding data than it was with respect to "run2" and "run3". The simulation using the run4 nudging configuration and the Shin-Hong PBL scheme ("run5") produced the smallest wind speed bias among the four sensitivity tests.

Figure 18 is a plot of Trial 308 Van 1 and Van 4 measured concentrations and the predicted ground-level concentrations using the version of WRF using the Shin-Hong PBL scheme which is referenced as WRF simulation C49.

It is immediately observed that there is significant improvement in the agreement between predicted and measured concentration in this figure as compared to Figure 18. HYSPLIT predictions based on WRF run5 improve the general agreement from a rough factor of ten to approximately a factor of 5 underprediction. The improvement in predictability demonstrated in Figure 18 is a direct consequence of the improved WRF numerical weather simulation.

Based on a NOAA/ARL observational study, at Cape Canaveral, to evaluate National Weather Service (NWS) predicted surface shear stress and TKE, a modification to the WRF predicted TKE fields was implemented within the HYSPLIT modeling system. NOAA/ARL conducted this meteorological study when additional high-precision sonic anemometers were installed at 10 m above the local displacement height, the height of local dense vegetation, on Tower 110. Tower 110 was one of the anchor points used during the MVP program for elevated tracer releases including a point of reference for blimp location for Trial 308.

Figure 19 plots a regression of WRF-HRRR predicted TKE versus measured TKE for the Tower 110 station. WRF-HRRR refers to the NWS implementation of the High-Resolution Rapid Refresh (HRRR) model. WRF-HRRR is an operational implementation of WRF-ARW V3.8.1+ (www.rapidrefresh.noaa.gov/hrrr). As shown, the observed TKE from Tower 110 is roughly 2 times that would be predicted by WRF-HRRR. This increased TKE was used to modify the near-field WRF boundary-layer predictions.

Figure 20 presents a plot of HYSPLIT predicted concentrations, using the modified TKE profiles, at nominally 18.75 to 19.25 km downwind against the measured ground-level concentration observed by Vans 1 and 4 which made transects of Route A1A during Trial 308. However, adjusting the calculated TKE to match observations does not improve the transport and diffusion model skill beyond a factor of 3-4 underprediction. The additional turbulence simply translates into more horizontal plume spread; while, the increased vertical turbulence does not translate into significant plume transport to the ground that would increase ground-level concentrations.

With the release of HYSPLIT version 5 (referenced herein as the latest version), there is an additional scheme available to parameterize vertical turbulence. This scheme, called Hanna, is described as letting the vertical Lagrangian time scale vary in space and time. The calculated scale is based on the vertical velocity variance estimated in the vertical turbulence scheme. Figure 21 continues the form of previous plots of measured concentration at 18.75 to 19.25 km downwind versus HYSPLIT predicted concentration based on the Hanna Lagrangian Time Scale (LTS) algorithm. As shown there appears to be some improvement between predicted and observed concentration levels. Although visual inspection of Figure 21 would suggest better agreement between predicted and measured concentrations, the difficulty in establishing a comparison metric would still suggest a factor of 3-4 underprediction. Further analysis, beyond this demonstration study, is needed to establish a more robust skill score.

Figures 22 and Figure 23 provide an alternative visual presentation of model skill demonstrated with HYSPLIT ground-level concentration predictions.

Figure 22 plots HYSPLIT C49 predicted versus measured concentrations between 18.75 and 19.25 kilometers downwind of the release point. This corresponds to the same data presented in Figure 18. However, the predicted and measured data are limited to points where bearing from the release point is restricted between 180 degrees azimuth and 210 degrees azimuth. Ground-level Gaussian concentration distributions are quite evident for both predicted and measured concentration fields. From Figure 22, a rough 5-degree azimuth difference in plume centerlines is estimated. It is also interesting to note that the horizontal shape or distribution for each data set is similar. An estimate of plume width based on Figure 22 is quite close to the Turner Workbook D-stability Gaussian sigma-y (Turner, 1970).

Figure 23 is a similar plot for HYSPLIT run5 Hanna LTS ground-level predicted concentrations. Again, defining an average concentration for measured concentrations is difficult. However, HYSPLIT predictions can be estimated as a factor of three lower than measured.

4.1.2 Trial 308 Release Height Concentration Evaluation

Aircraft SF_6 measurements are difficult to relate to model calculations since measurements represent spatial and temporal snapshots of a temporally and spatially varying released plume. However, these observations do provide a qualitative assessment of transport and diffusion model skill. Shown in Figure 24 is a plot of elevated plume predicted and observed concentrations for Trial 308. HYSPLIT predictions represent the average concentration within a layer between 200 m and 300 m AGL. Aircraft measurements are those data points along the flight path crossing the plume roughly 19km downwind of the source and with a bearing following the tracer plume centerline. Aircraft sampled points are annotated with assigned sampling height.

Qualitatively, there is good agreement between predicted and measured concentrations within the limits imposed by sampling protocols. A visual inspection again suggests a rough 5-degree azimuth difference between the measured and predicted plume centerline.

4.2 Trial 309 Evaluations

As previously stated, due to limited vertical mixing there were no reported ground-level concentrations measured by mobile sampling vans for Trial 309. Sampling routes, based on a forecasted western track for the Trial 309 release, were not correctly positioned to detect the released tracer. Although several sampling routes potentially were positioned to transect the plume, van sampling start times led to missing the ground plume or that airborne concentrations were below detection limits for the SF_6 samplers.

However, a comparison of HYSPLIT predicted ground-level concentrations for Trial 309 with predictions for Trial 308 in Figure 25, following the previous centerline analyses, does suggest well-behaved numerical simulations with analogy to comparison of measured ground-level concentrations. Accordingly, there is no reason to not suggest similarity for Trial 309, since both trials saw strong steady northeasterly winds through each tracer release.

5.0 Summary and Conclusions

The NOAA/ARL HYSPLIT model was exercised for both MVP Trials 308 and 309 using a suite of WRF outputs in which 5 nudging options were imposed of the numerical weather predictions. HYSPLIT transport and diffusion model predictions were compared to the Trial 308 measured tracer measurements between 18.75 and 19.25 km downwind of the elevated release point. Differences between predicted and measured concentrations were determined to decrease from a factor-of-ten underprediction to roughly a factor of three with the transition of WRF from no observational nudging to nudging with both surface and upper-air measurements.

The best agreement between Trial 308 measurements and transport and diffusion model predictions was observed with WRF nudging Run 5 and the HYSPLIT Version 5.0 transport and diffusion model with TKE turbulence routines and Hanna Lagrangian time scale algorithms. Although Trial 309 reported no measurable ground-level concentrations; given the similarities in atmospheric conditions between Trial 308 and Trial 309, there is no reason to suspect significant dissimilarities in model skill scores.

Review of the circumstances of the two releases considered reveals that the probability was high that the releases occurred at a time when local turbulence intensity was potentially limited. Additional consideration of the local and regional atmospheric turbulence fields should provide insight into the vector transport details of the resulting elevated plumes, necessarily affecting ground level concentrations as were observed.

While only a limited set of tracer releases were evaluated, it can still be concluded that given the appropriate numerical weather simulation, the 1996 MVP study is capable of providing a rich database for evaluation, verification, and validation of numerical modeling of the potential release of hazardous or radioactive materials within the environment of the CCAFS. Examination of MVP datasets in the light of developing PBL understanding is expected to result in enhancements to the atmospheric transport and diffusion formulations applied to elevated releases.

6.0 References

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Table 1 Summary of MVP Tracer Session Three Trials 308 and 309

Trial Number	308	309
Date	May 1, 1996	May 1, 1996
Tracer release time (EDT)	06:01 to 08:31	11:15 to 13:33
Release Latitude	28° 34.19’	28^0 33.82’
Release Longitude	80° 35.210’	80^0 36.360’
Release Height above MSL (m)	305	610
Approximate Mixing Depth (m)	427 - 549	549 - 792
Wind Direction (degrees azimuth)	015	070
Wind Speed (m/s)	11	9
Tracer release Location	Over Tower 110	Over Schwartz Static Test Roads/West edge of Banana River Lagoon
Study Observation	Transport SSW over Banana River Lagoon. Vans measured tracer on E-W causeways. Plume steady, with vertical aligned (i.e., surface and aloft) tracer centerline maxima.	Limited vertical mixing. Vans did not detect tracer at ground level. Aircraft detected plume within a shallow vertical layer.

Table 2 Sampling summary for Trial 308 and Trial 309

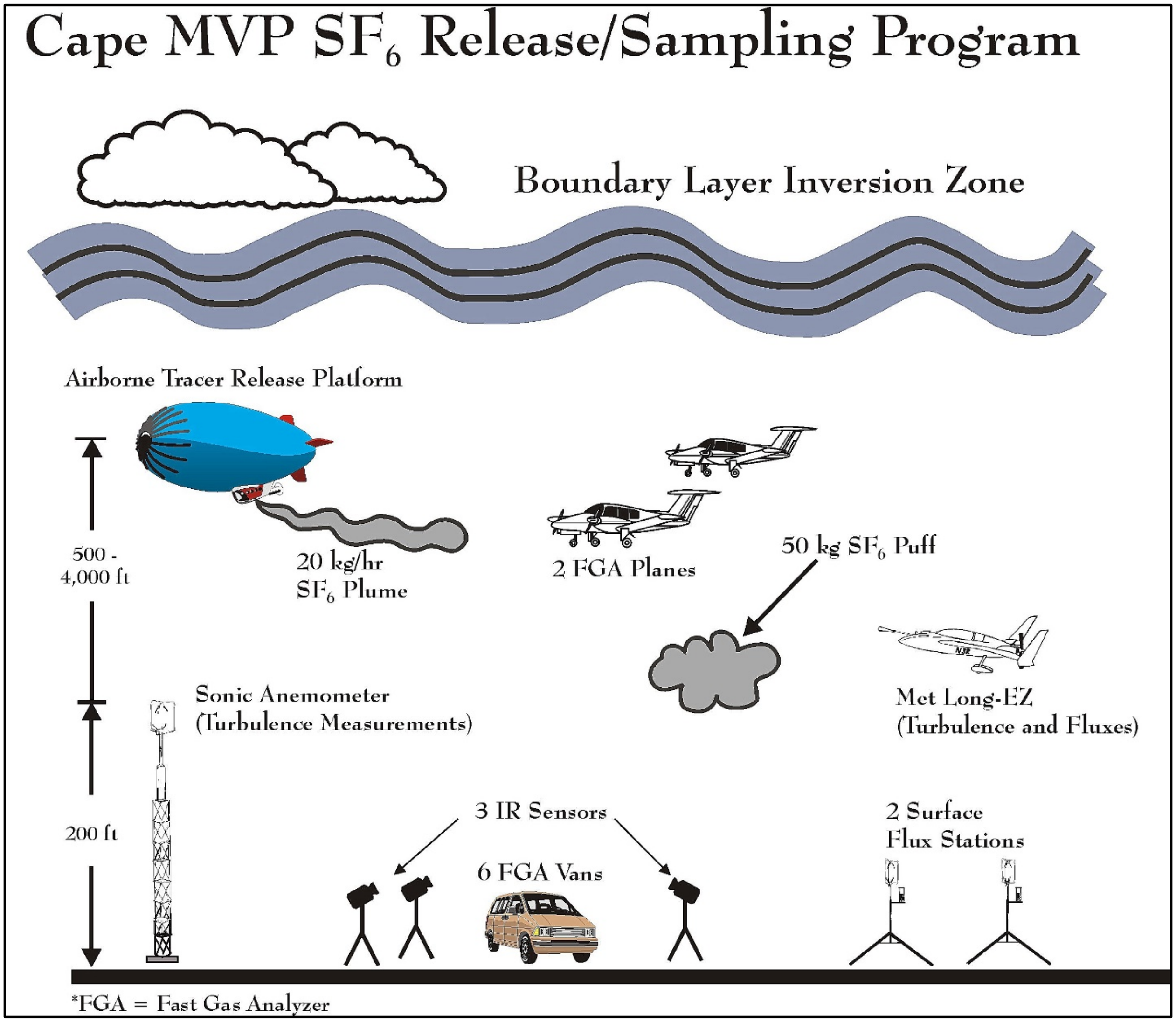
Sampling Platform	Trial 308 (hits)	Trial 309 (hits)
Van 1	12	0
Van 2	Not Available	Not Available
Van 3	15	0
Van 4	27	0
Van 5	32	0
Van 6	0	0
Aircraft 1	23	9
Aircraft 2	Not Available	Not Available

Table 3 Levels of WRF modeling

Designation	Description
Cape 1	NARR Database
Cape 2	NARR Database plus MVP surface observations
Cape 3	NARR Database plus MVP surface and upper air observations (3-Hour update)
Cape 4 – run1	NARR Database plus MVP surface and upper air observations (1-Hour update)
Cape 4 – run2	Based on Cape 4 and increasing nudging coefficient for the wind to 8.0e-4
Cape 4 – run3	Based on Cape 4 and increasing nudging coefficient for the wind to 1.2e-3
Cape 4 – run4	Based on run3 and decreasing the vertical weighting of surface data
Cape 4 – run5	Based on run4 and using Shin-Hong PBL scheme instead of MYNN 2.5-level scheme

Table 4 List of HYSPLIT and WRF simulations for Trials 308 and 309

Test	WRF Simulation	HYSPLIT
1	NARR database	SVN 951
2	NARR Database + MVP surface observations	SVN 951
3	NARR Database + MVP surface and upper air observations	SVN 951
4	NARR Database + MVP surface and upper air observations	Version 5
5	NARR Database + MVP surface and upper air observations	Version 5
6	NARR Database + MVP surface and upper air observation (“run 1”)	Version 5
7	NARR Database + MVP surface and upper air observations (“run 2”)	Version 5
8	NARR Database + MVP surface and upper air observations (“run 3”)	Version 5
9	NARR Database + MVP surface and upper air observations (“run 5”)	Version 5



Depiction 1 Schematic of tracer release, concentration measurement, and supplemental atmospheric measurement platforms for USAF-sponsored Model Validation Program experiments in Cape Canaveral area. NOAA/ARL/ATDD graphic, based on an earlier sketch by R. F. Kamada.

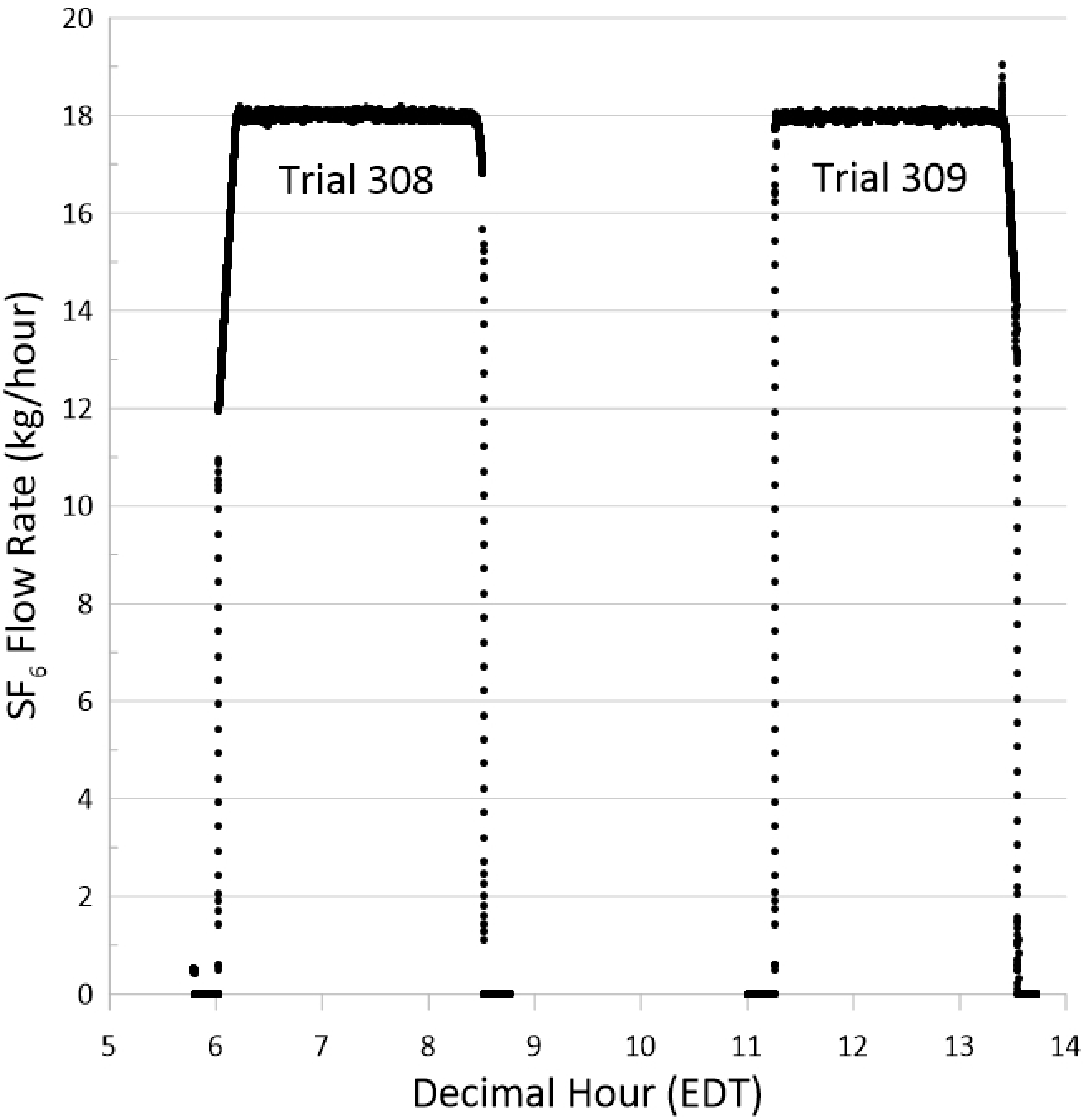


Figure 1. SF_6 flow rates from the blimp platform. Excursions in the release rate at release startup and end are inconsequential.

Note: Plotted time is the recorded sampling time given as a fractional hour based on local daylight savings time (EDT).

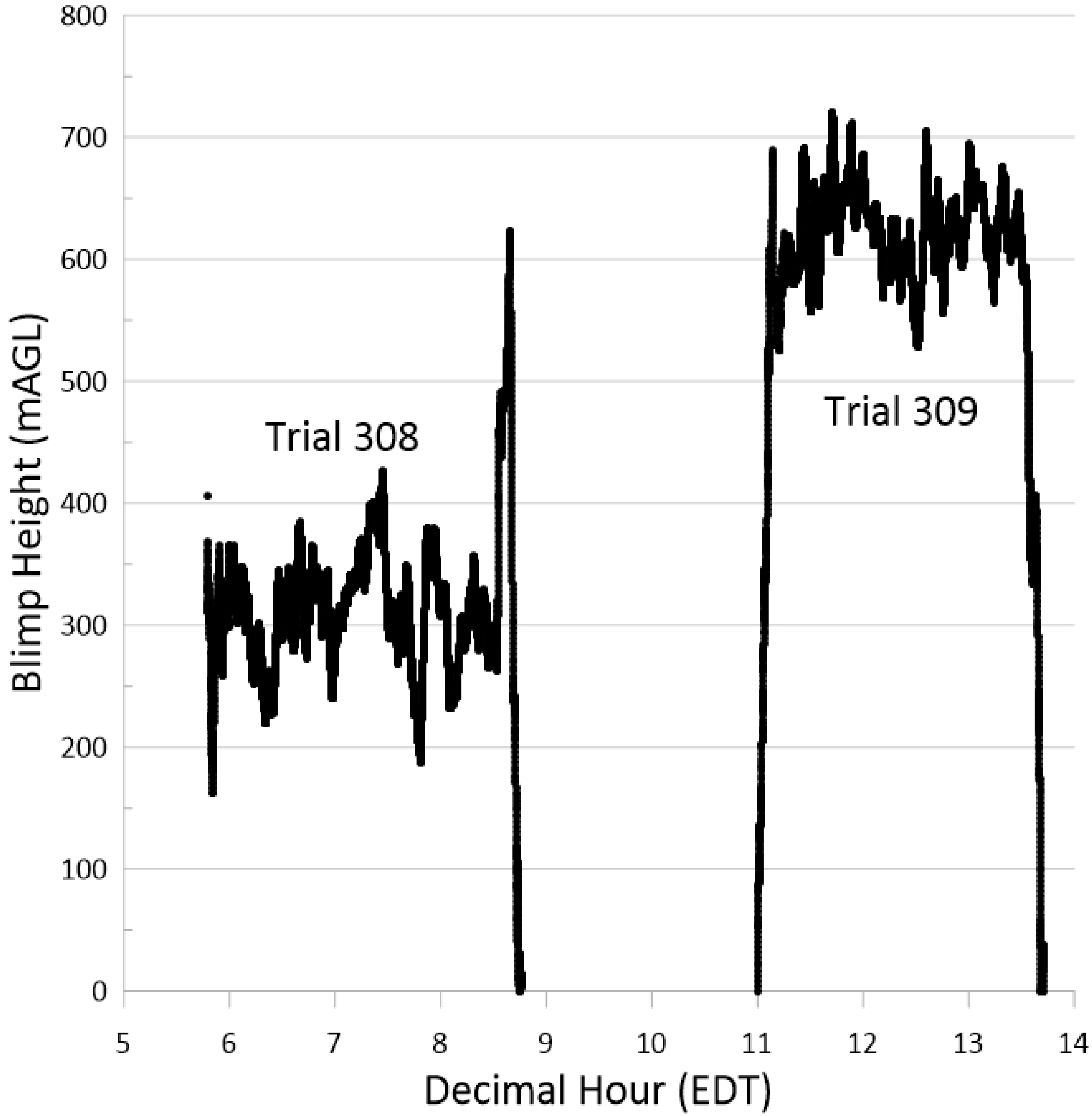


Figure 2. Blimps heights over the tracer release period for Trial 308 and Trial 309. Excursion in blimp altitude at the beginning and end of the sample release period are inconsequential.

Note: Plotted time is the recorded sampling time given as a fractional hour based on local daylight savings time (EDT).

Figure 3 Flight path of blimp for tracer releases Trial 308 and Trial 309.

Note: Actual flight paths only deviate by tens of meters from the targeted release position.

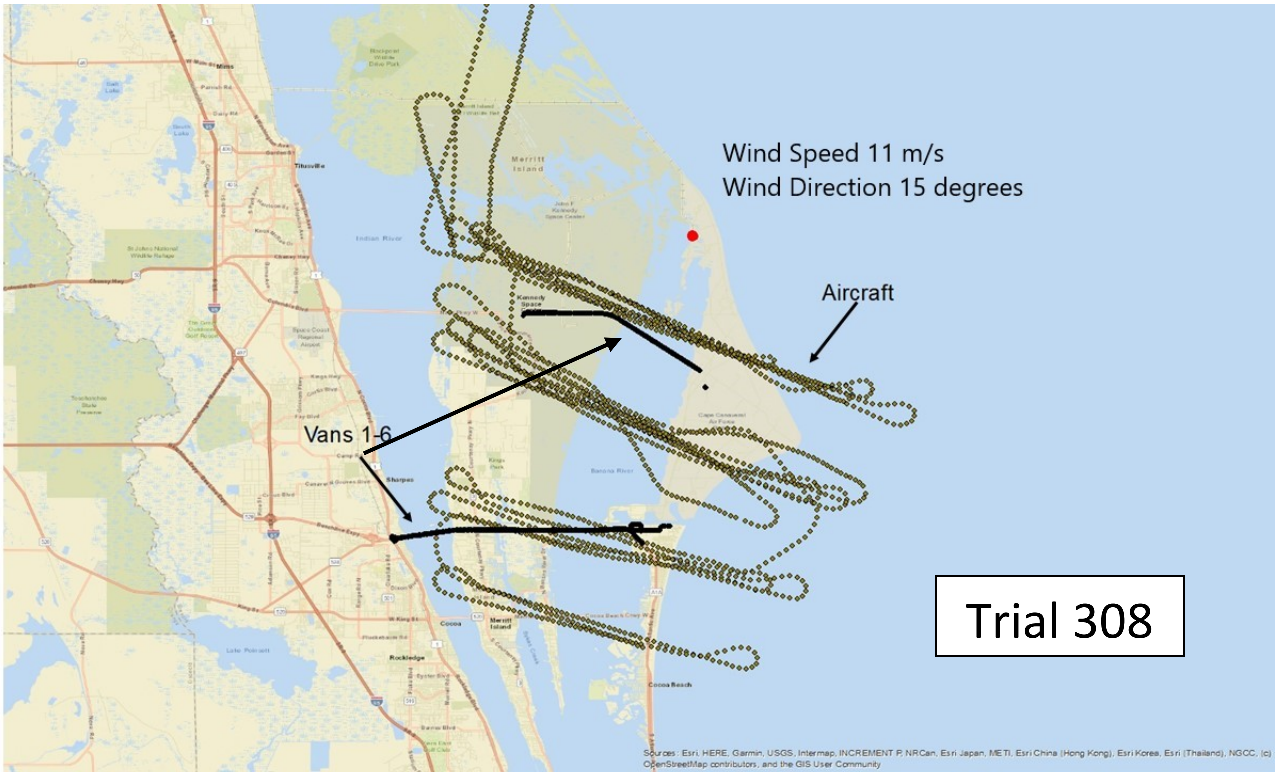


Figure 4 Trial 308 sampling tracks for instrumented vans and aircraft

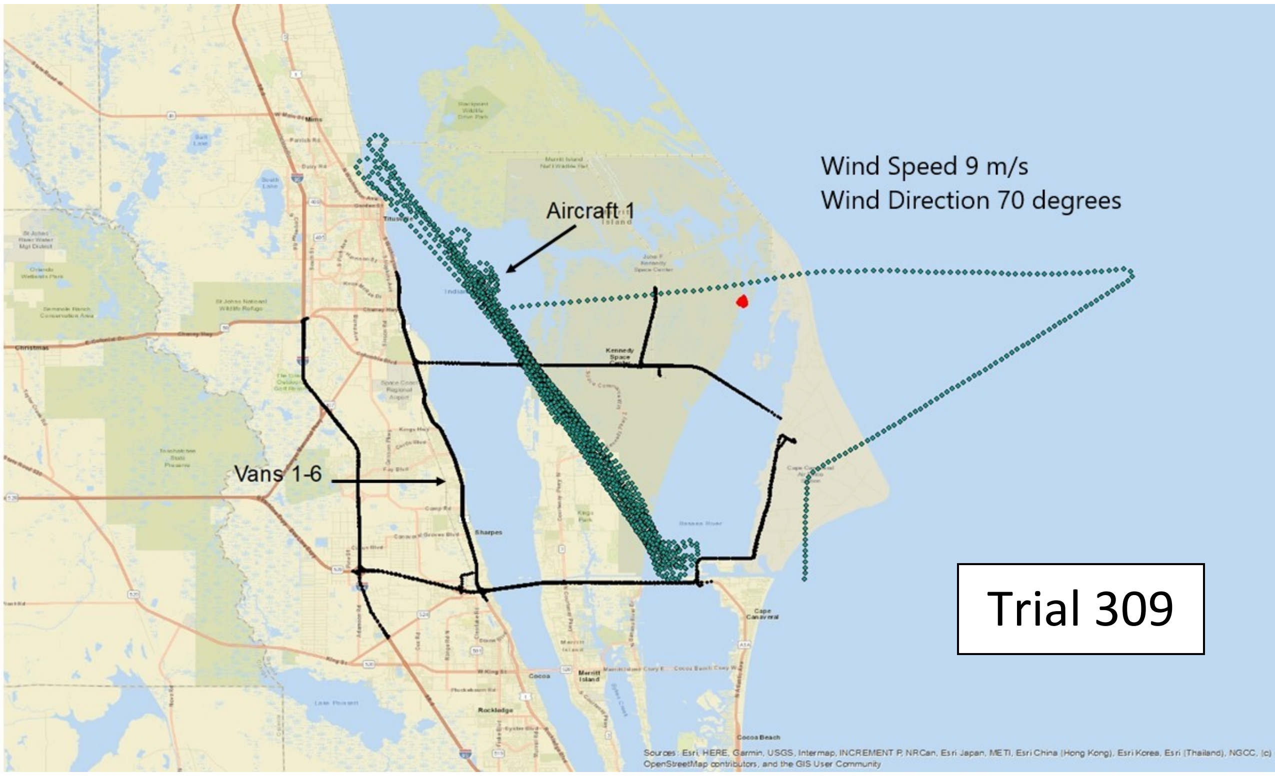


Figure 5 Trial 309 sampling tracks for instrumented vans and aircraft.

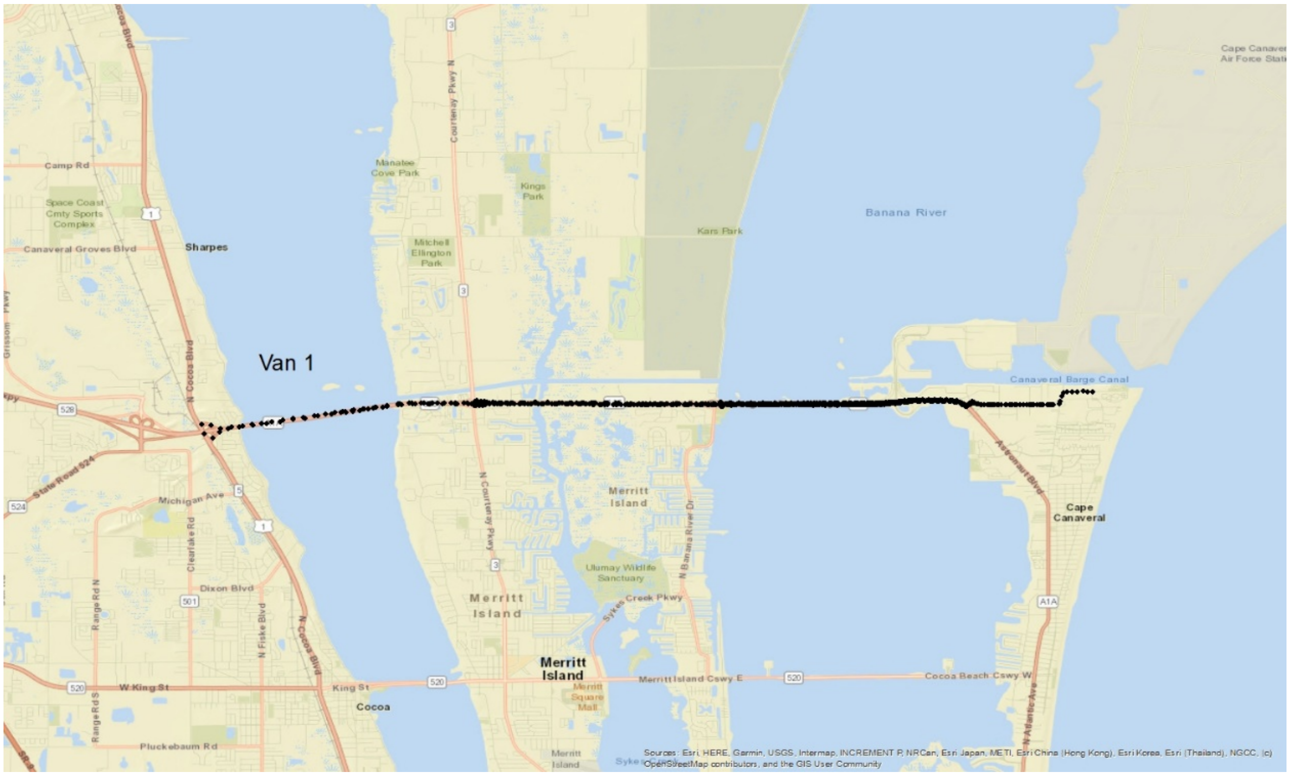


Figure 6 Trial 308 Van 1 and Van 4 sampling route. Plotted data points indicate sampling position (latitude and Longitude) assigned to recorded measured concentration for Van 1.

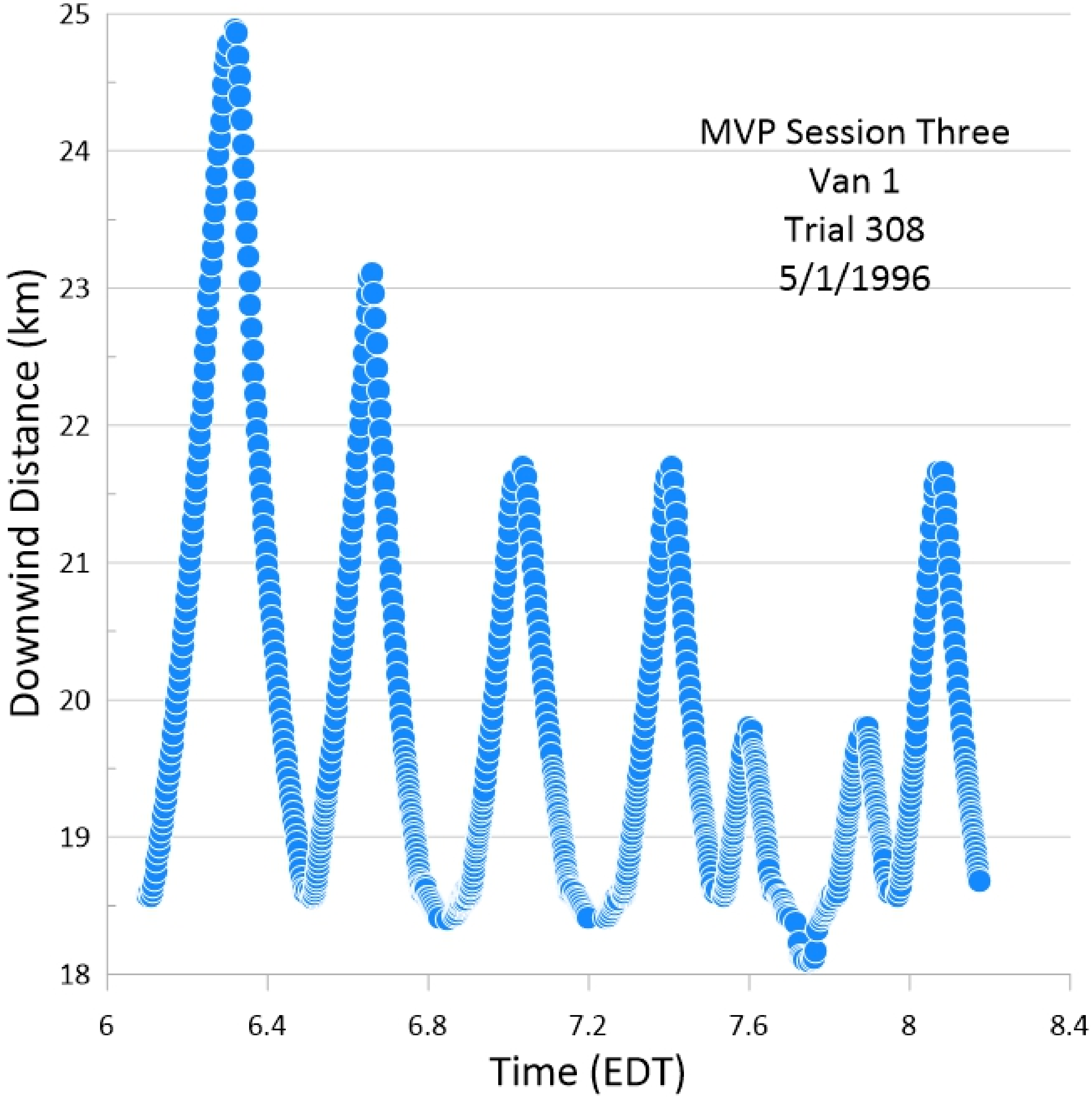


Figure 7 Sampling transects for Van 1 along the Indian River Lagoon Scenic Highway A1A/528. Plotted time is the recorded sampling time given as factional hour based on local daylight saving (EDT) time.

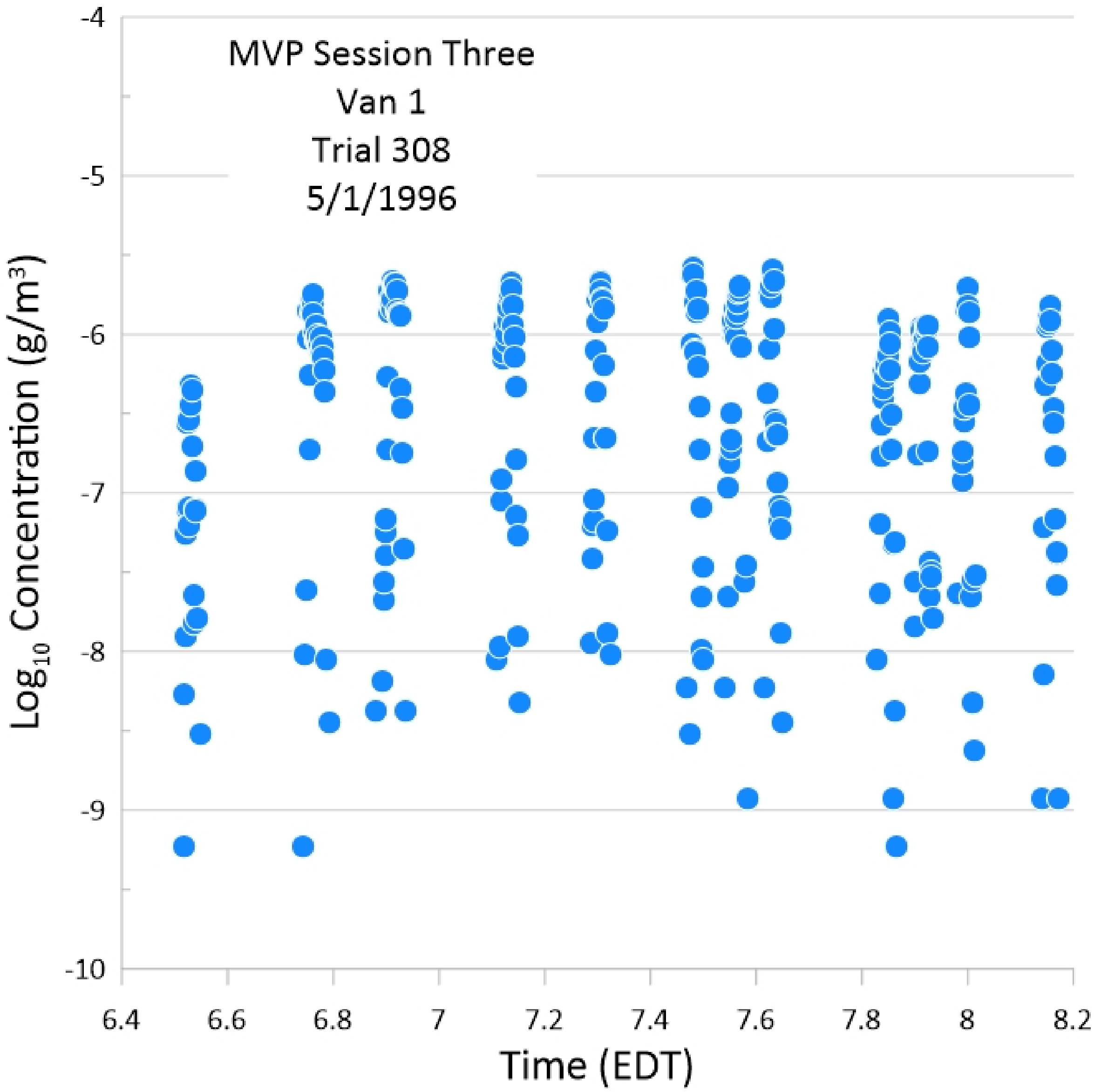


Figure 8 Ground-level SF6 concentration measured by Van 1 during Trial 308. Plotted time is the recorded sampling time given as factional hour based on local daylight saving (EDT) time.

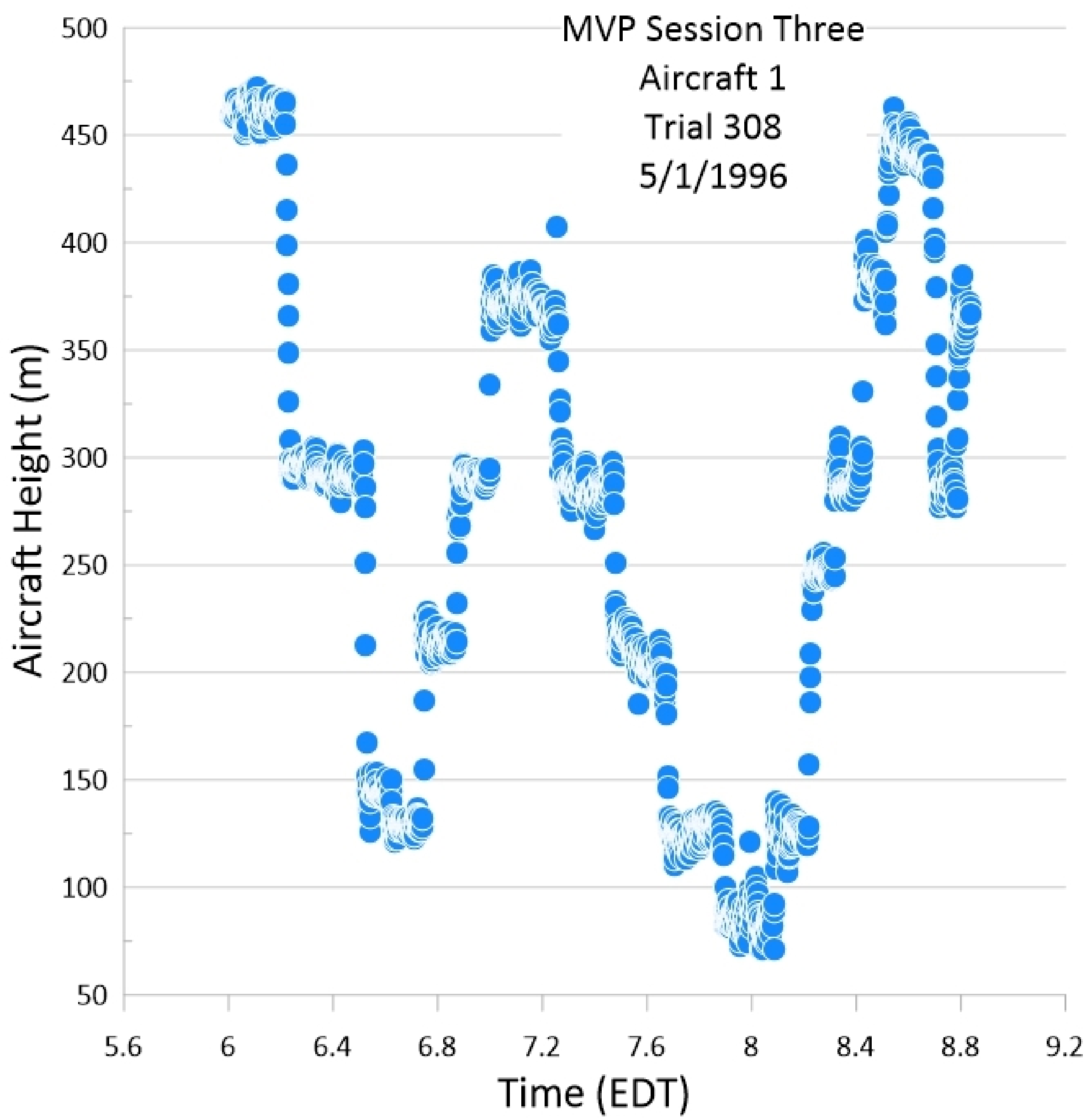


Figure 9 MVP Session Three Trial 308 aircraft sampling transects. Plotted time is the recorded sampling time given as factional hour based on local daylight saving (EDT) time.

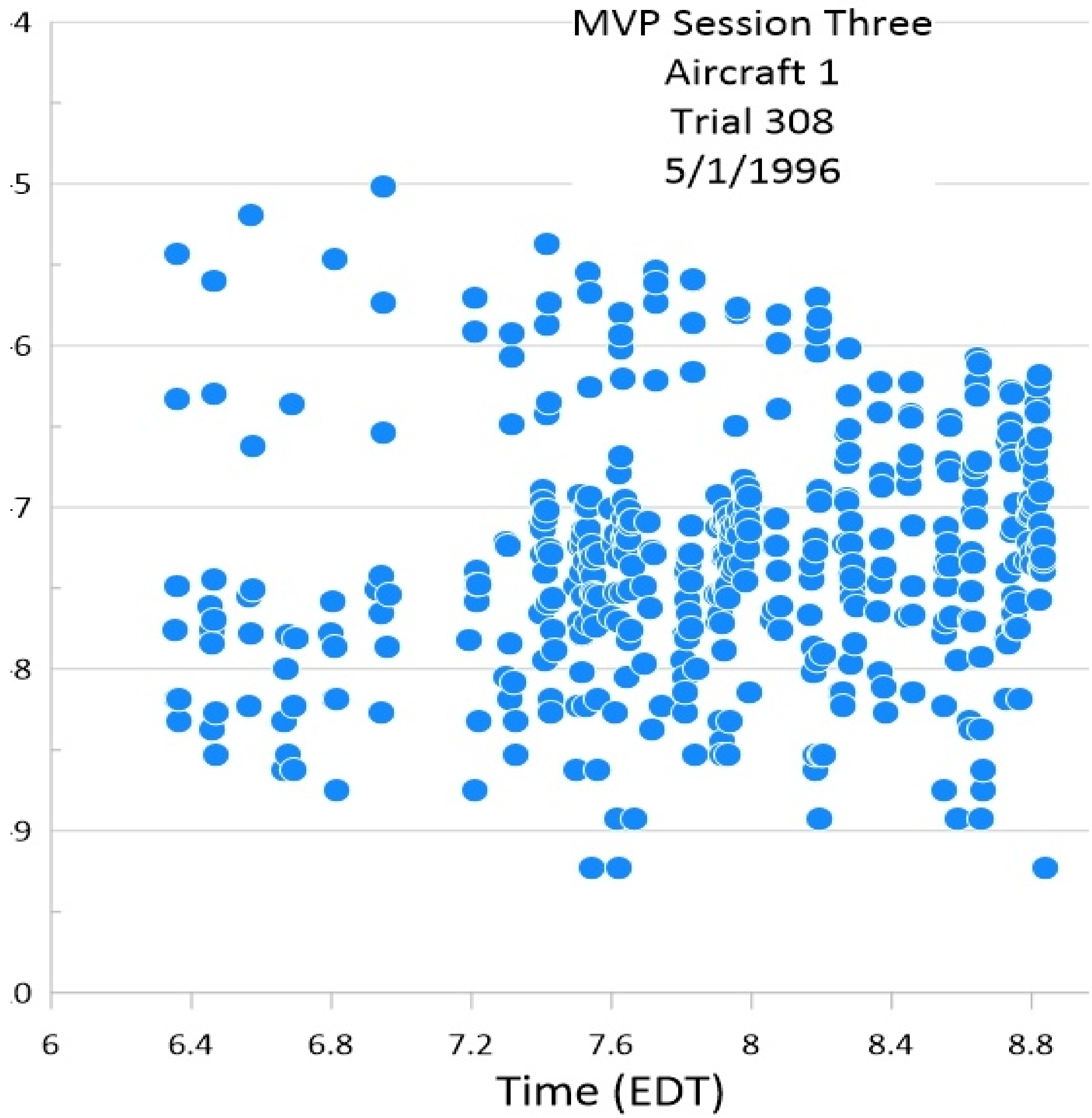


Figure 10 Measured airborne SF_6 concentrations measured by aircraft 1 during Trial 308. Plotted time is the recorded sampling time given as factional hour based on local daylight saving (EDT) time.

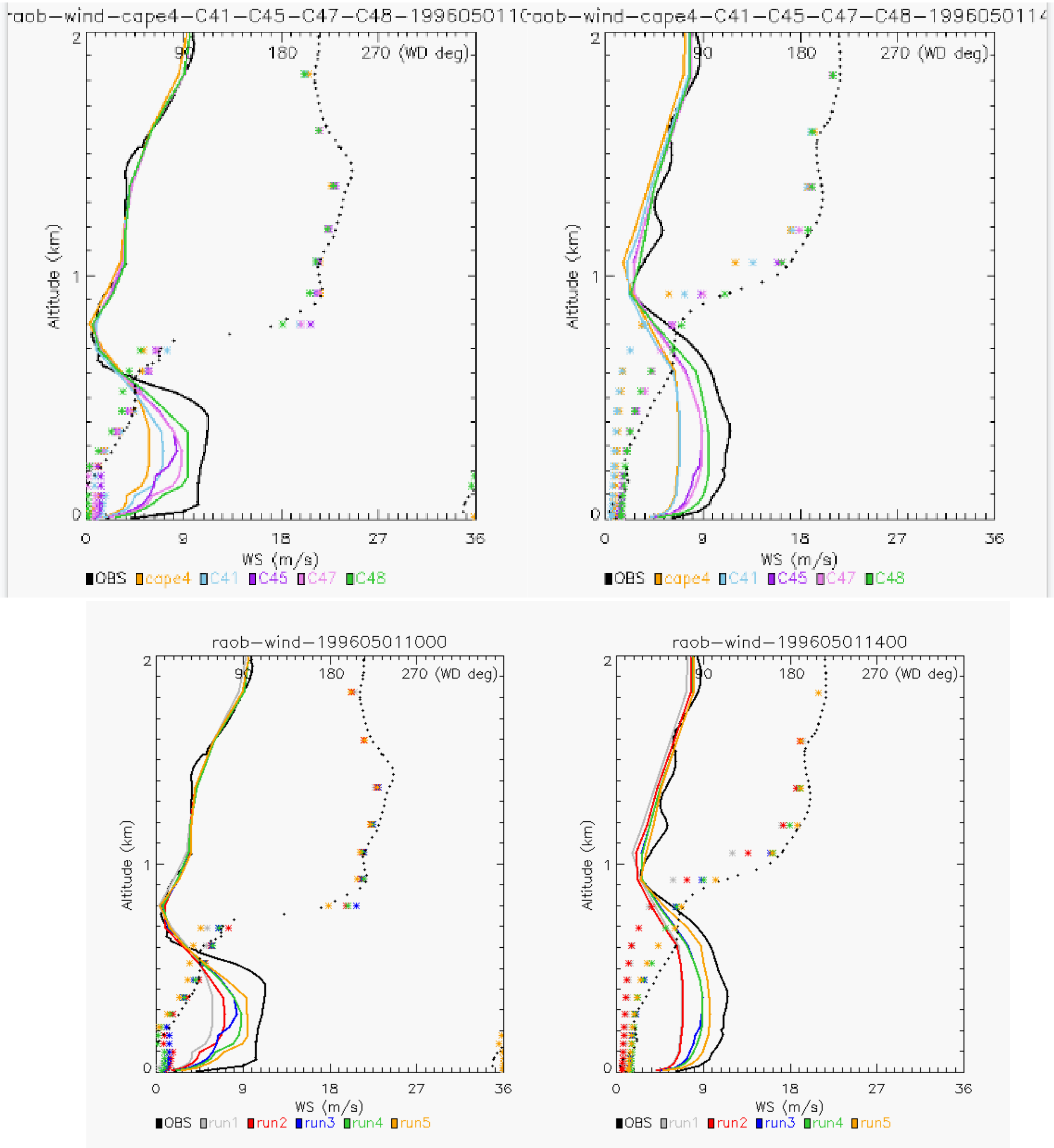


Figure 11 Vertical profiles of wind speed (solid lines) and wind direction (dotted lines) at 10 UTC (left panel) and 14 UTC (right panel) on May 1, 1996.

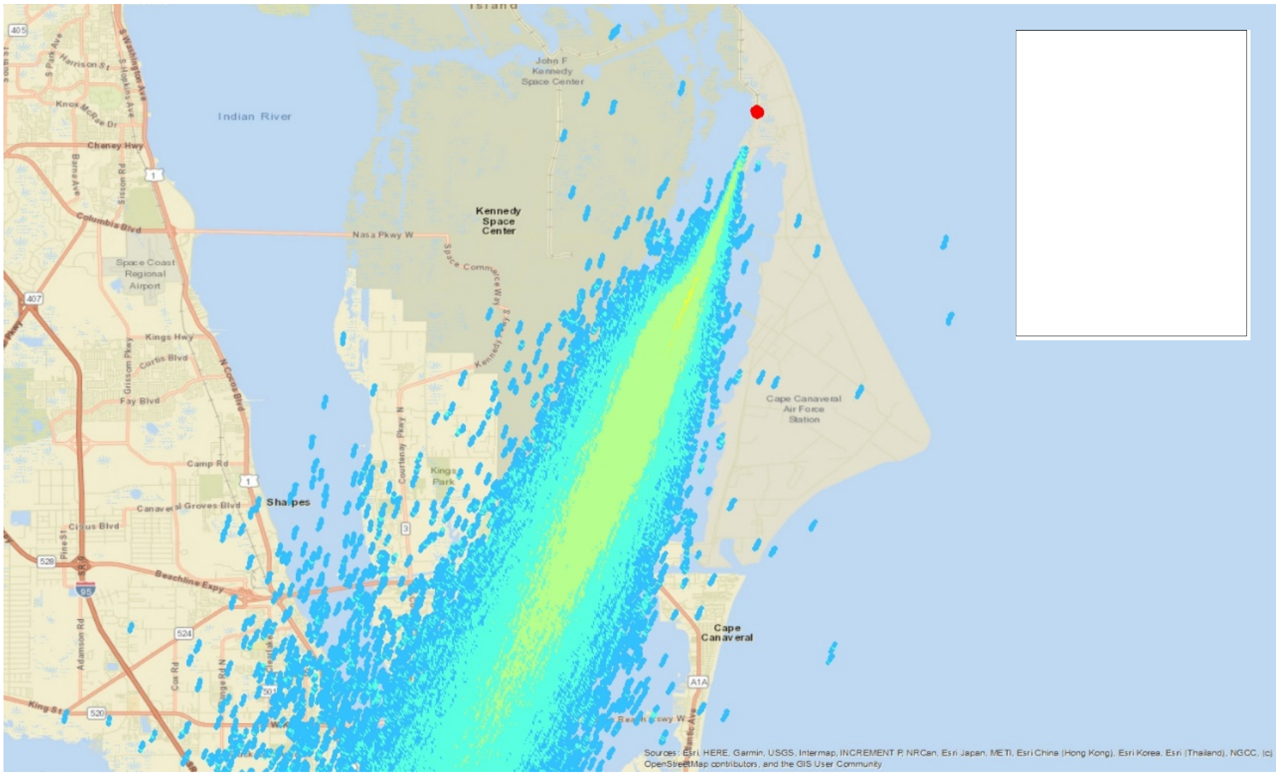


Figure 12 Trial 308 predicted ground-level concentration.

Note: For clarity of analysis and presentation the log_{10} concentration is mapped.

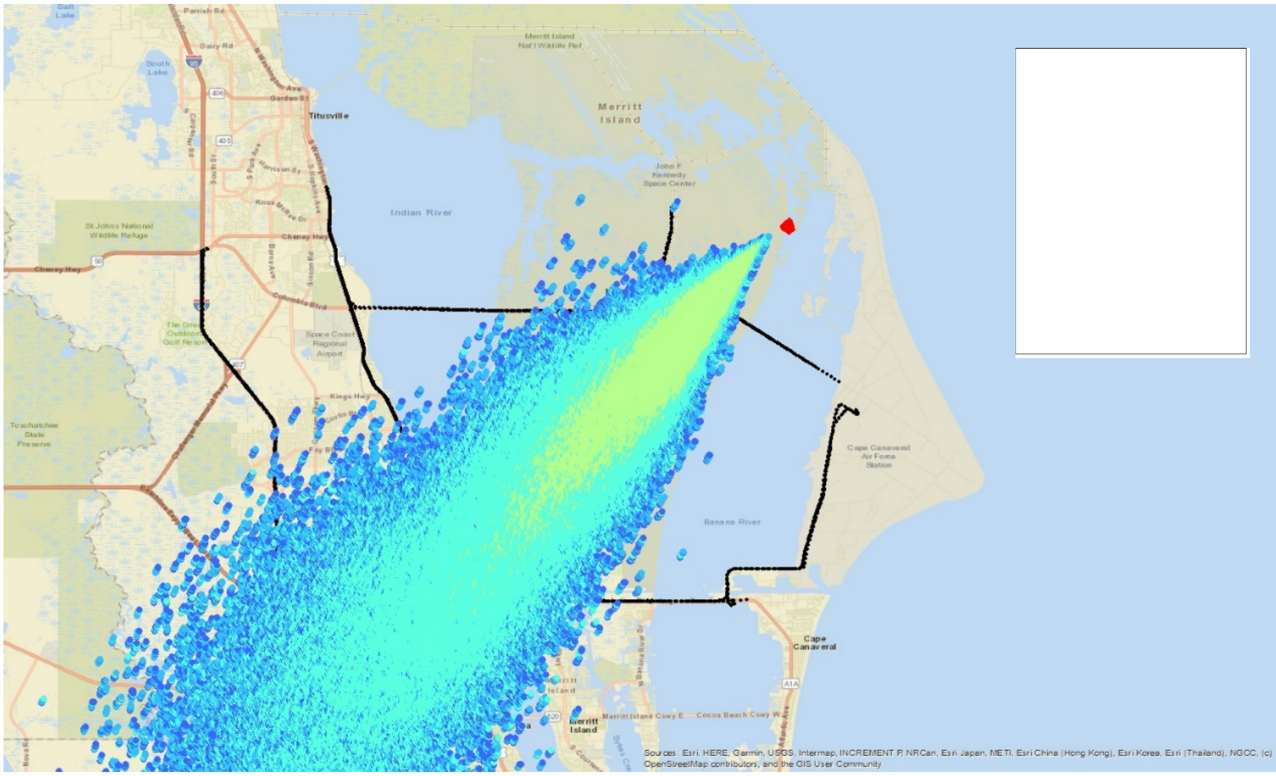


Figure 13 Trial 309 predicted ground-level concentration.

Note: For clarity of analysis and presentation the $\log_{10}$ concentration is mapped.

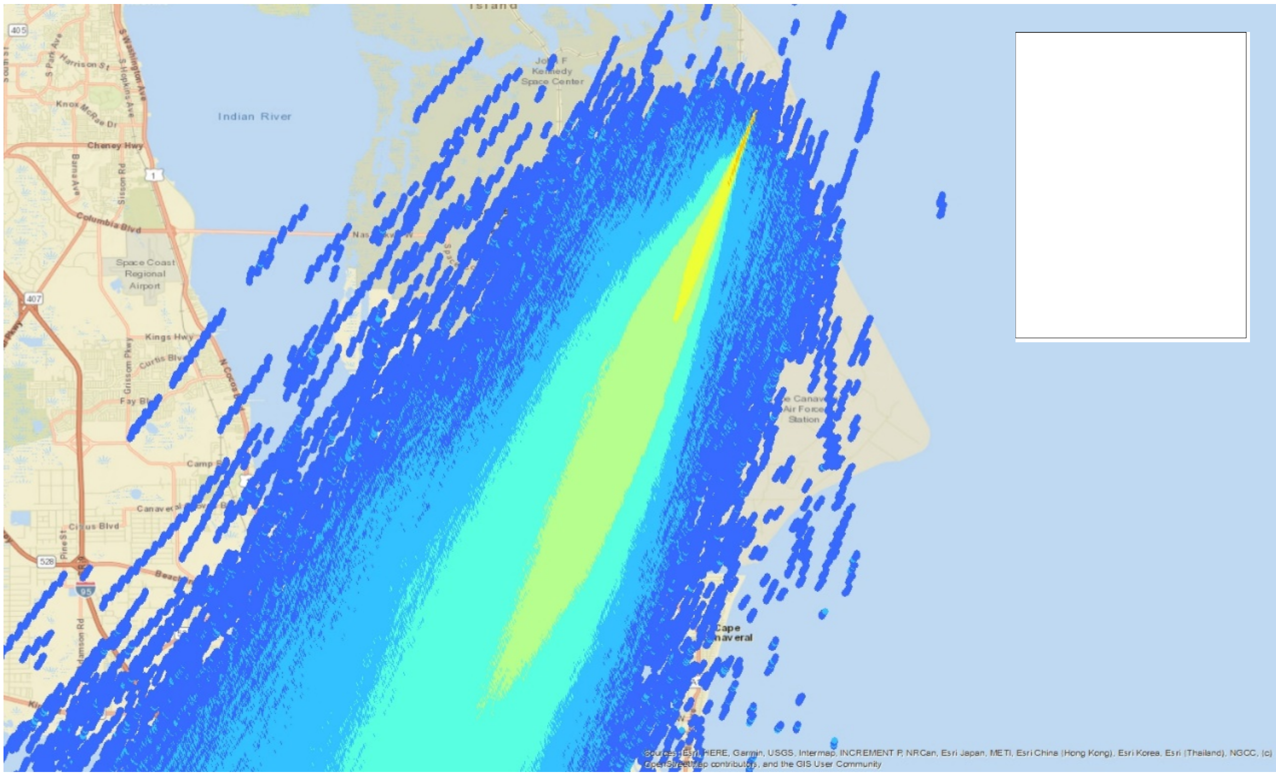


Figure 14 Trial 308 release height (305m) predicted airborne concentration.

Note: For clarity of analysis and presentation the $\log_{10}$ concentration is mapped.

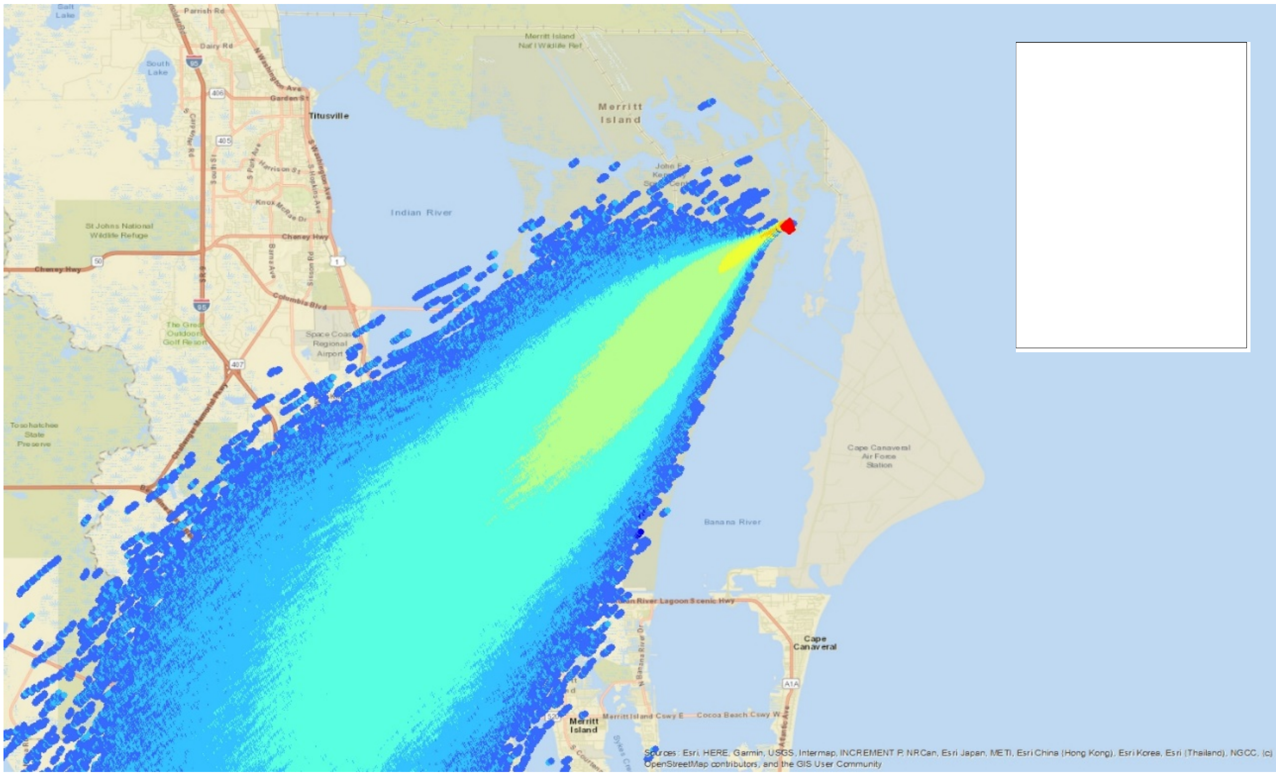


Figure 15 Trial 309 release height (610m) predicted airborne concentration.

Note: For clarity of analysis and presentation the $\log_{10}$ concentration is mapped.

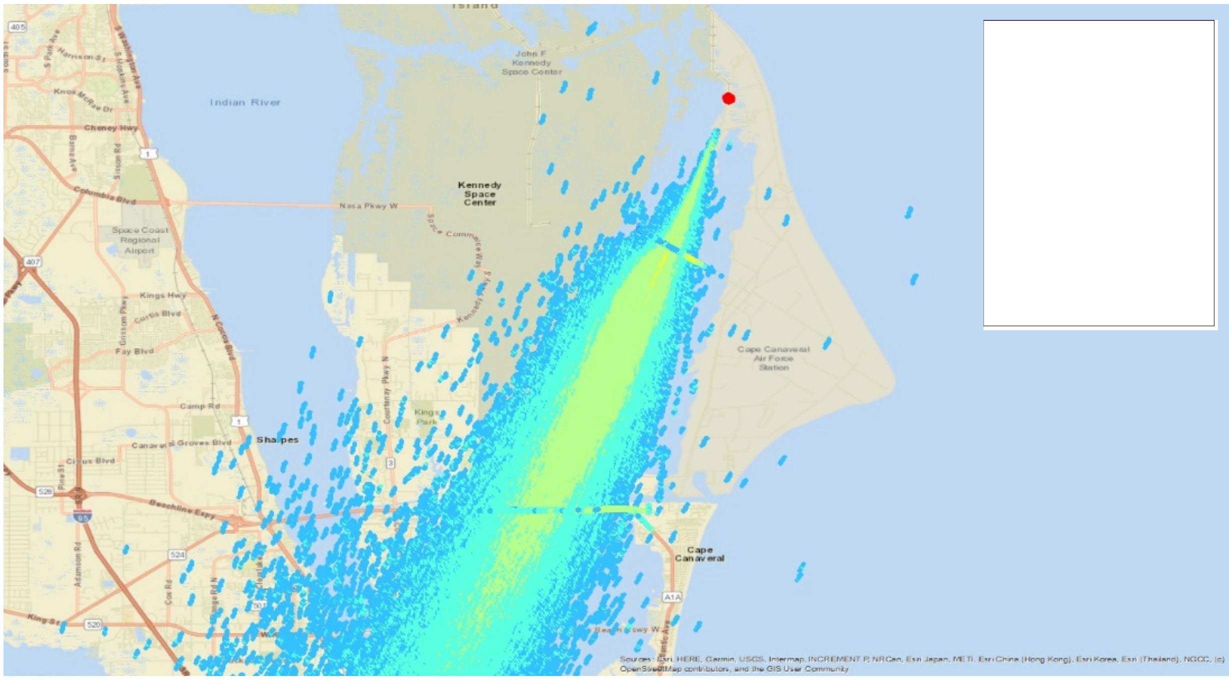


Figure 16 Trial 308 ground-level predicted concentrations coupled with measured concentrations following the designated Van sampling tracks.

Note: For clarity of analysis and presentation the $\log_{10}$ concentration is mapped.

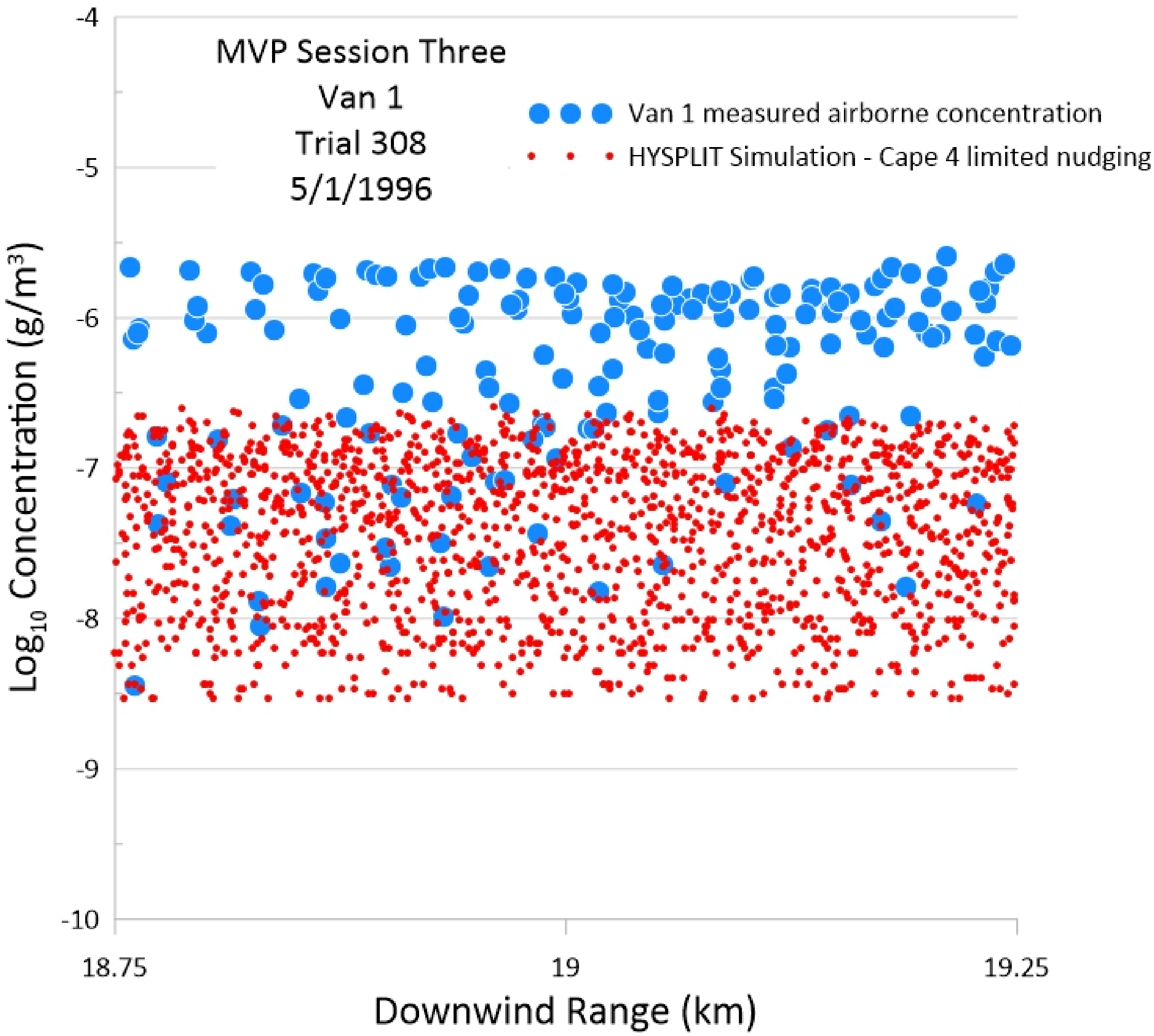


Figure 17 Trial 308 predicted and observed airborne concentration levels between 18.75 and 19.25 km downwind of the tracer release point, using Cape 4, basic nudging WRF output.

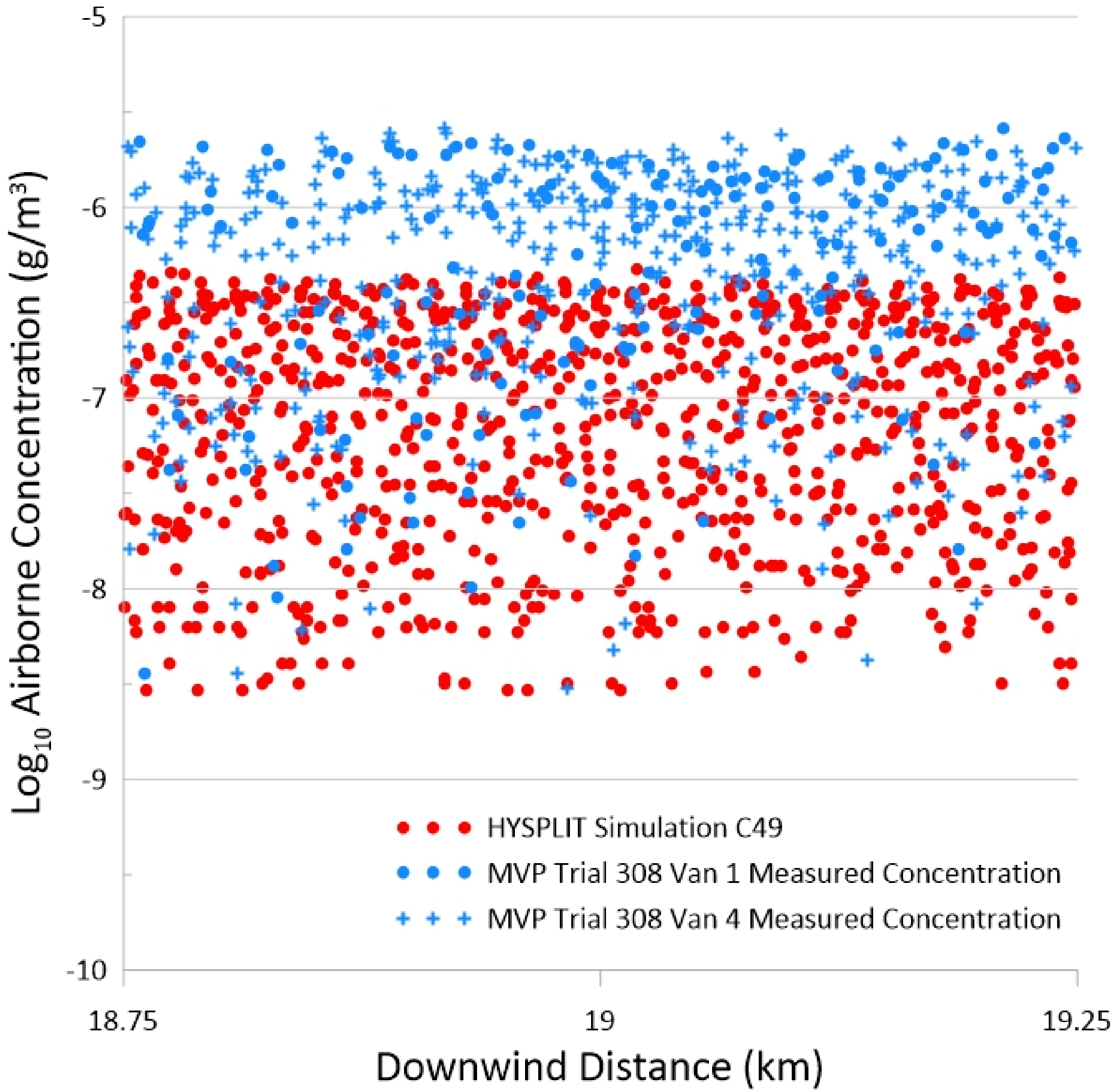


Figure 18 Trial 308 predicted and observed airborne concentration levels between 18.75 and 19.25 km downwind of the tracer release point using the C49 WRF simulation.

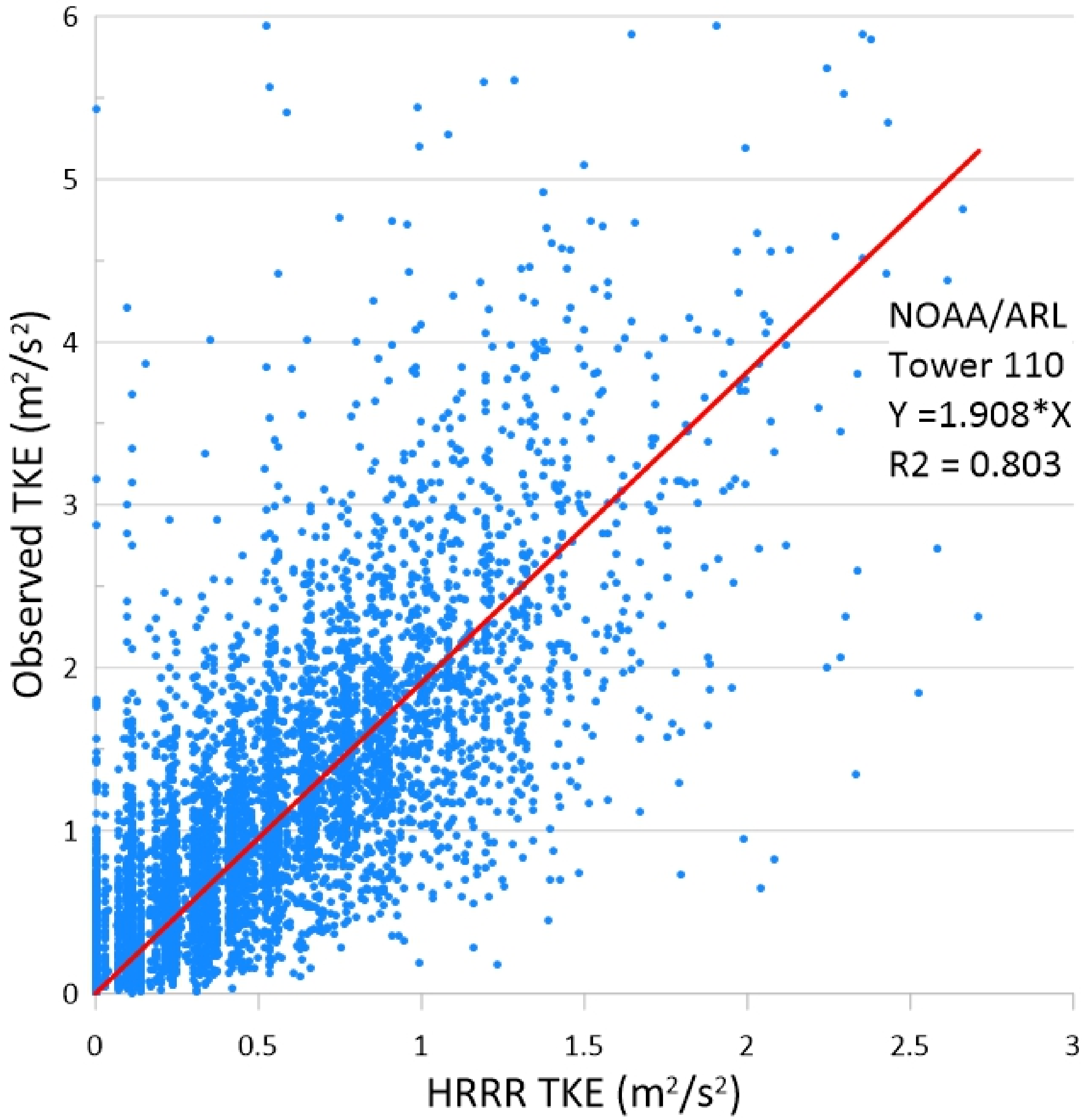


Figure 19 Regression analysis of measured TKE versus WRF-HRRR predicted TKE.

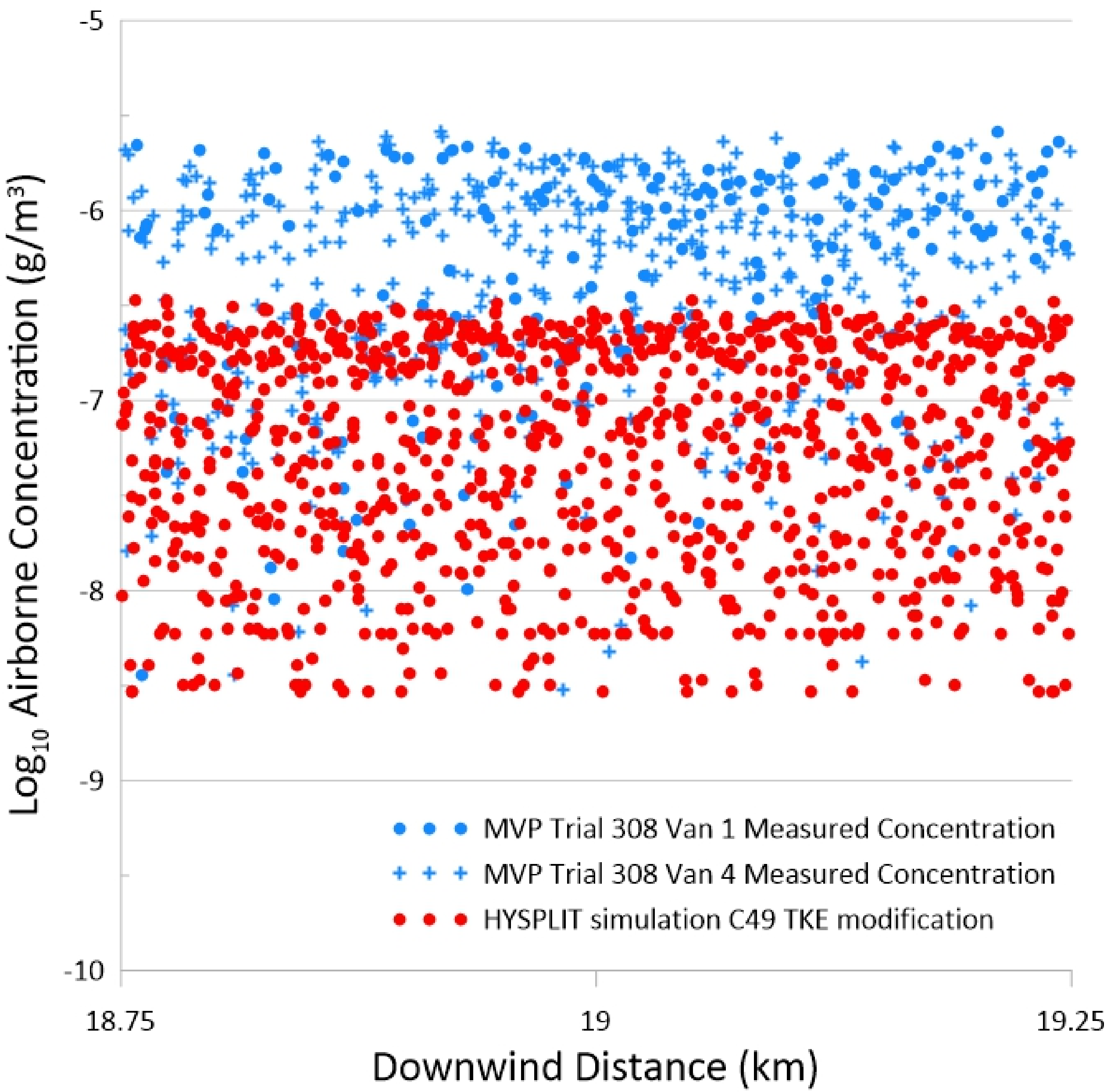


Figure 20 Trial 308 predicted and observed airborne concentration levels between 18.75 and 19.25 km downwind of the tracer release point using the C49 WRF simulation with TKE modifications.

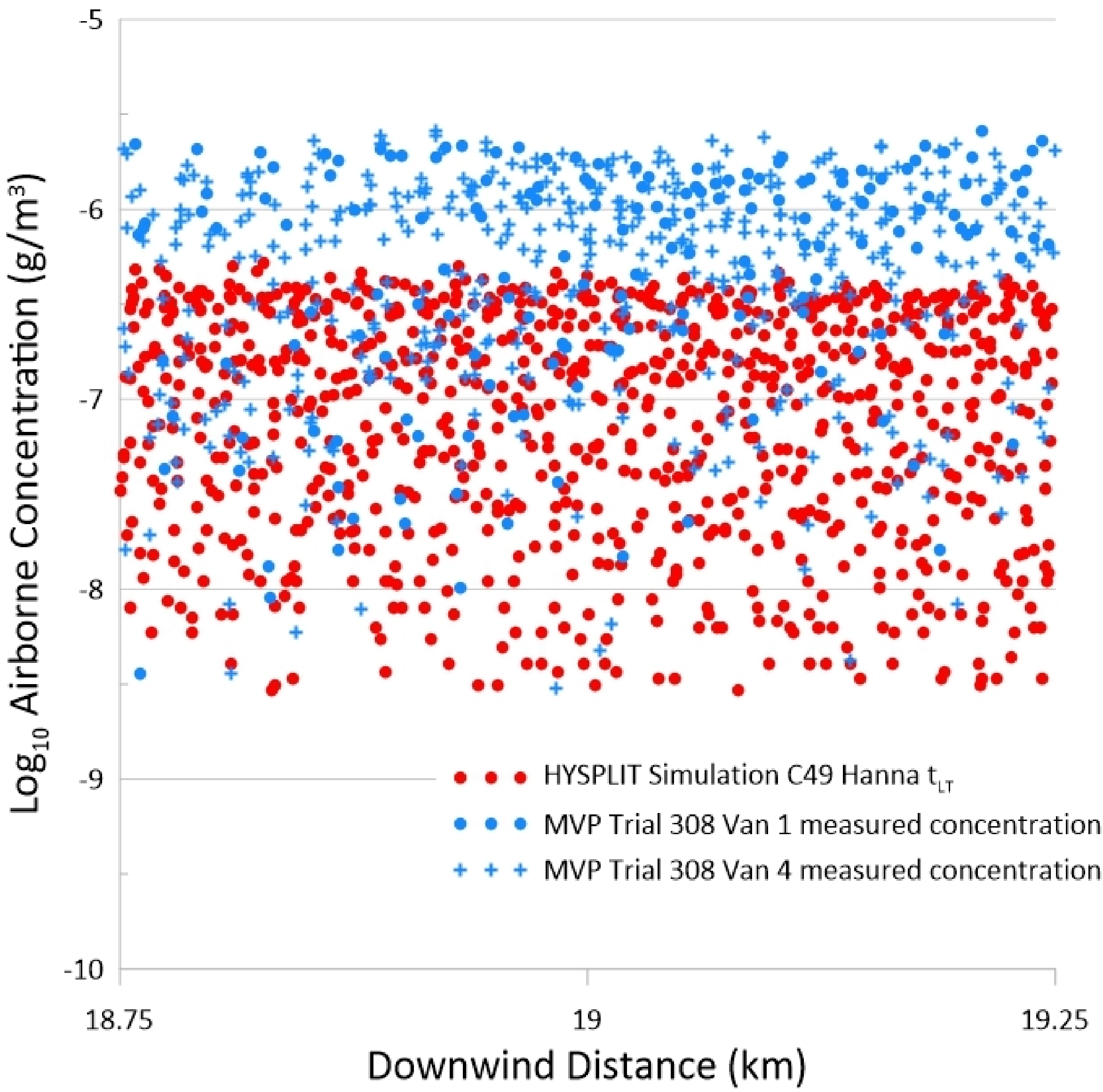


Figure 21 Trial 308 predicted and observed airborne concentration levels between 18.75 and 19.25 km downwind of the tracer release point using the C49 WRF simulation with TKE modifications.

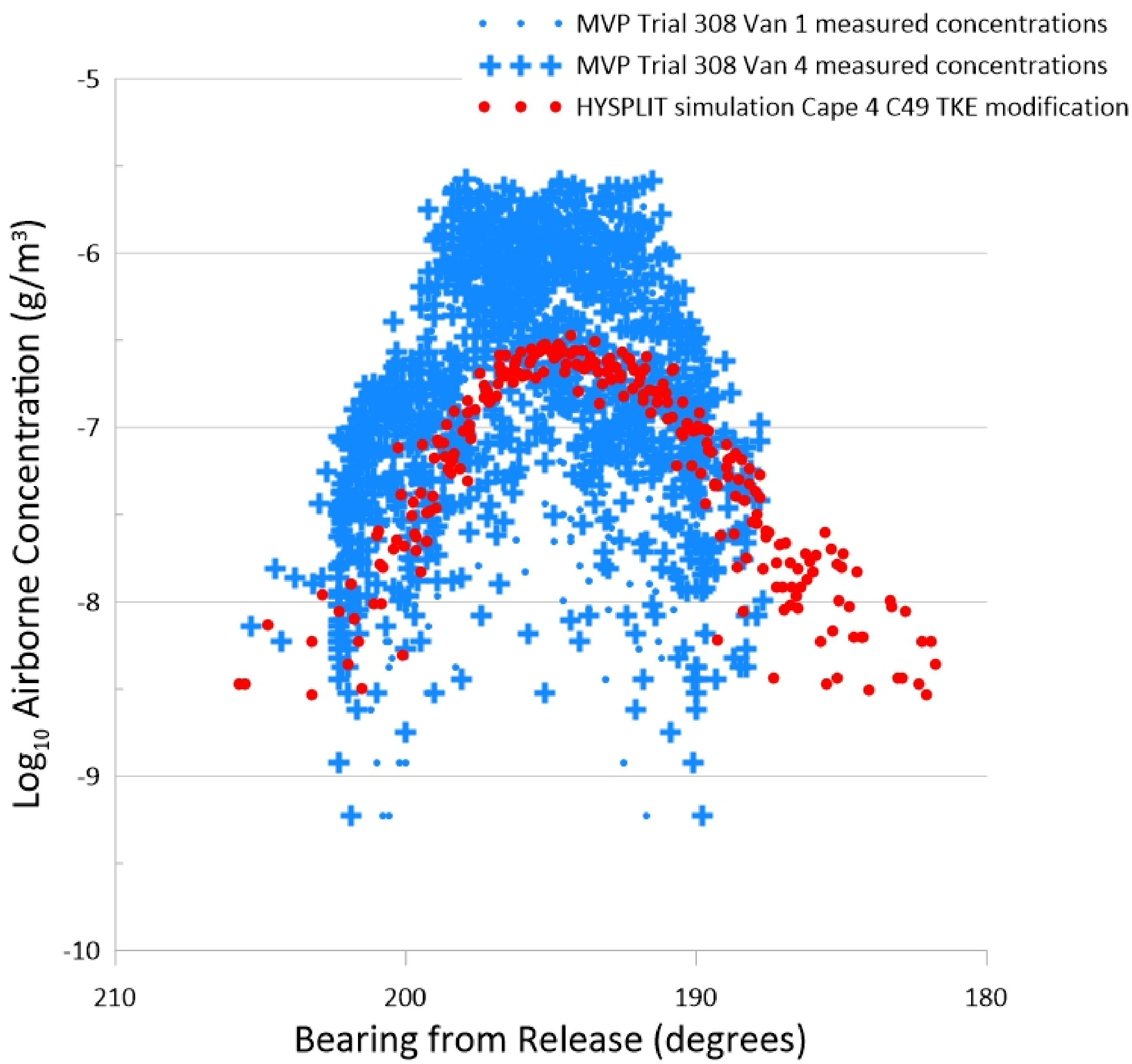


Figure 22 Trial 308 predicted and observed airborne concentration levels between 18.75 and 19.25 km downwind of the tracer release point using the C49 WRF TKE simulation

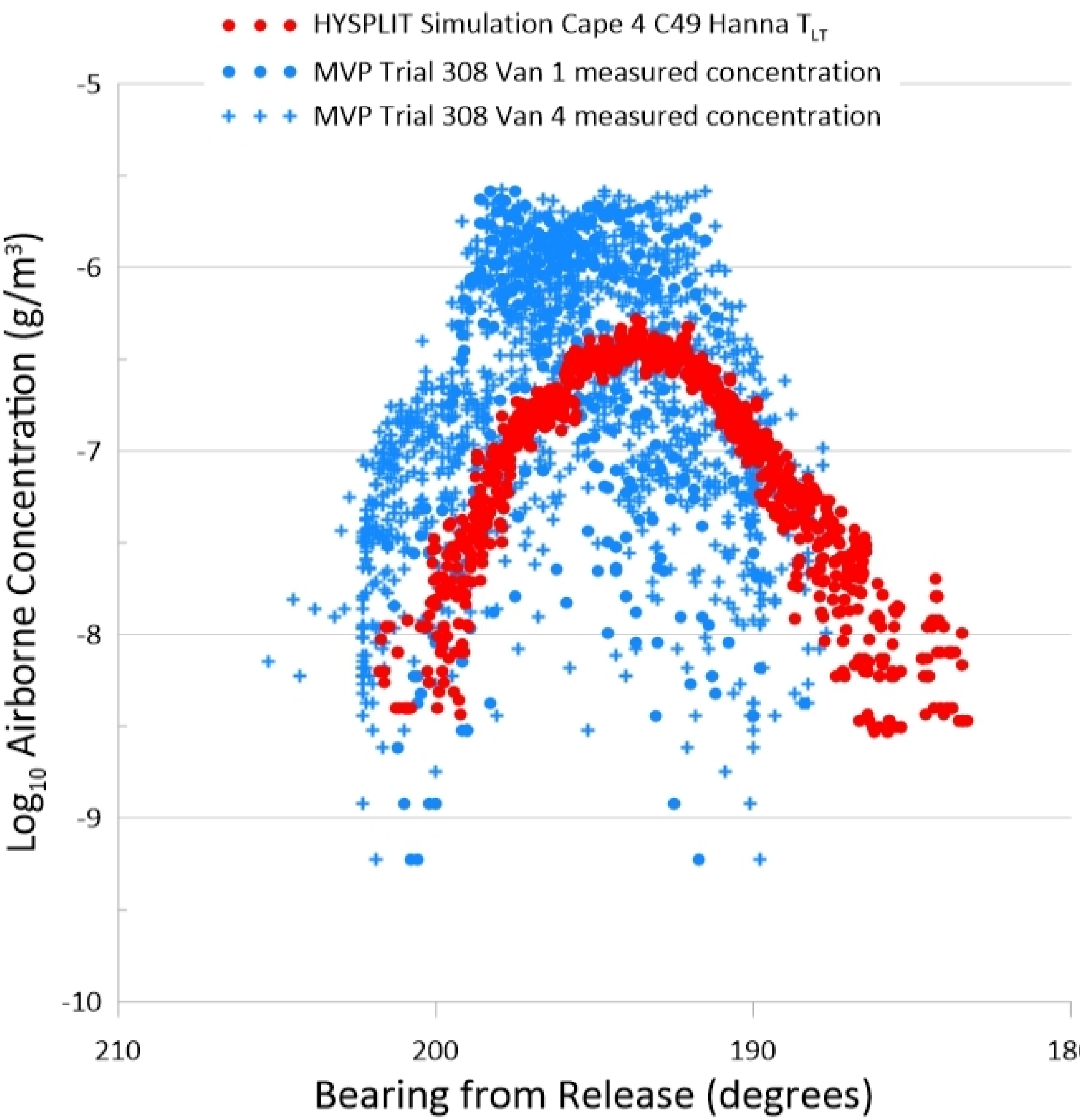


Figure 23 Trial 308 predicted and observed airborne concentration levels between 18.75 and 19.25 km downwind of the tracer release point using the C49 WRF Hanna T_{LT} simulation.

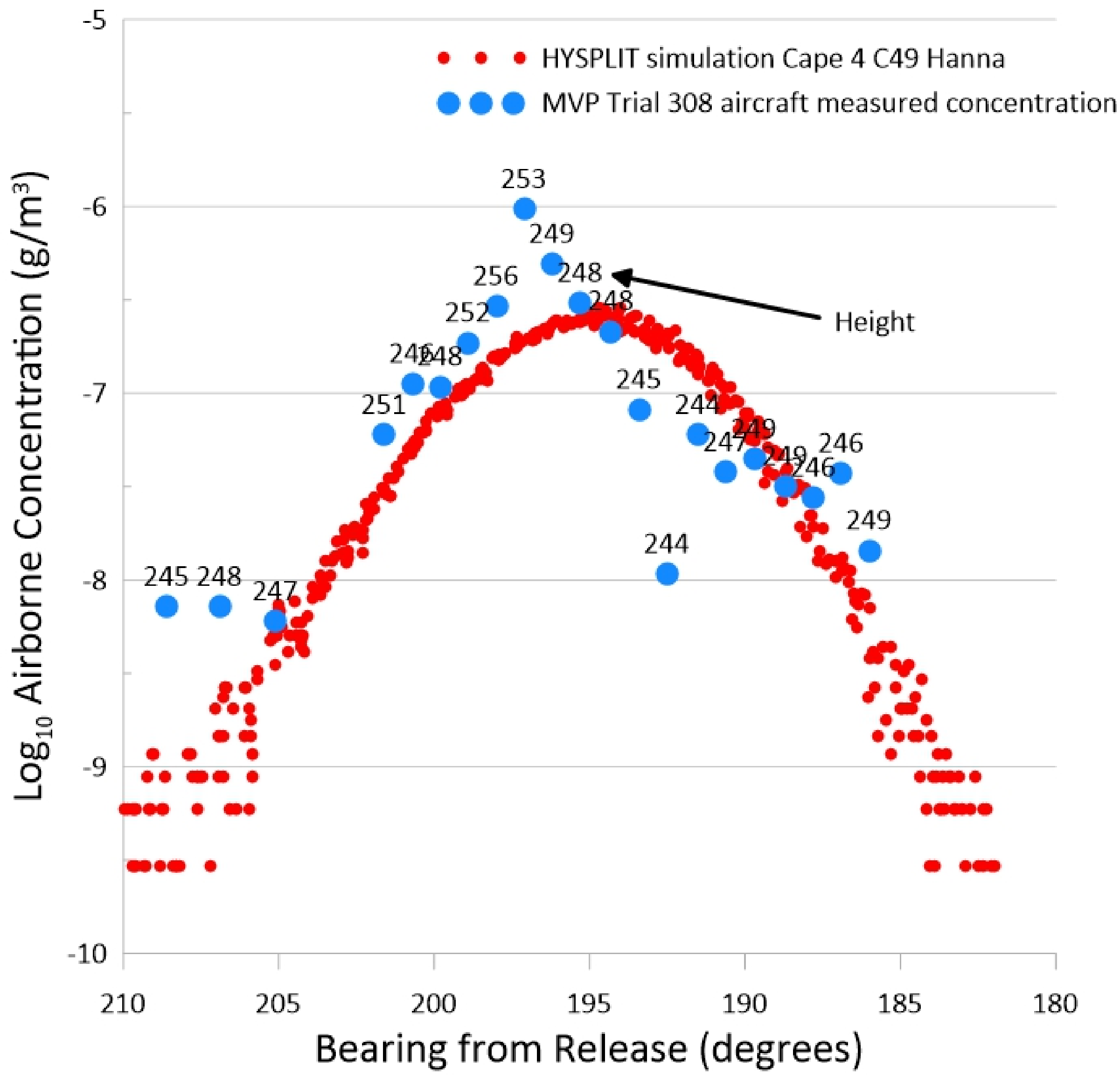


Figure 24 Measured and predicted airborne concentration for Trial 308 at 19km downwind of the release point

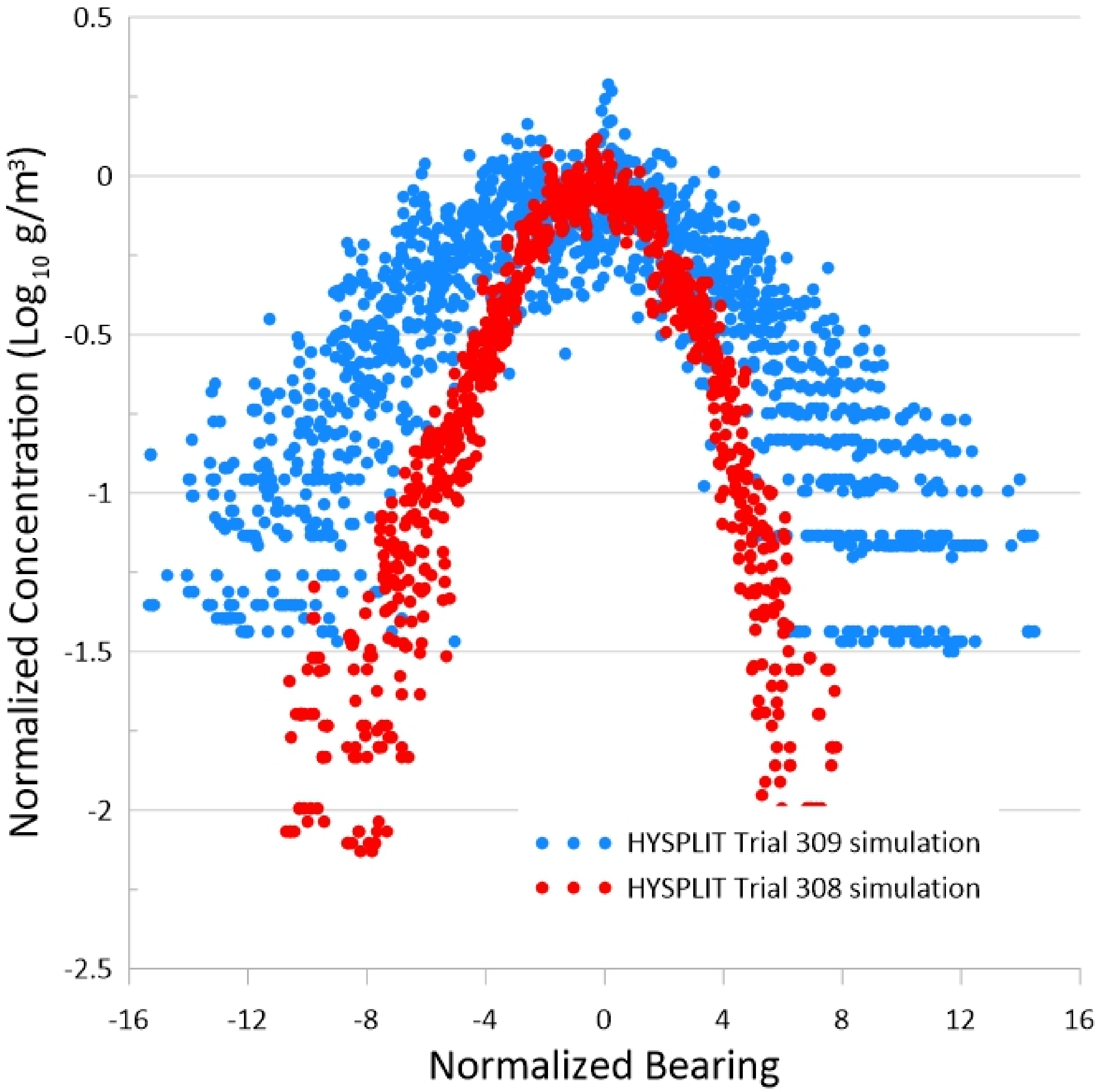


Figure 25 A comparison of HYSPLIT predicted ground-level concentrations for Trial 308 and Trial 309. Bearing from release point normalized by centerline bearing and concentration normalized by maximum concentration for both Trials